

The Structure of Some Crystals as Indicated by Their Diffraction of X-rays

W. L. Bragg

Proc. R. Soc. Lond. A 1913 **89**, doi: 10.1098/rspa.1913.0083, published 22 September 1913

References

Article cited in:

<http://rspa.royalsocietypublishing.org/content/89/610/248.citation#related-urls>

Email alerting service

Receive free email alerts when new articles cite this article - sign up in the box at the top right-hand corner of the article or click [here](#)

Lastly, though the absorption coefficient of the tungsten peak has not yet been satisfactorily measured, it may be doubtless supposed to be a little less than that of the A peak of platinum, since its wave-length is slightly less. A recent measurement of the latter quantity gives the value 35.5 and the absorption coefficient of the characteristic radiation of tungsten is given by Barkla as 33.

The Structure of Some Crystals as Indicated by their Diffraction of X-rays.

By W. L. BRAGG, B.A.

(Communicated by Prof. W. H. Bragg, F.R.S. Received June 21,—Read June 26, 1913.)

[PLATE 10.]

A new method of investigating the structure of a crystal has been afforded by the work of Laue* and his collaborators on the diffraction of X-rays by crystals. The phenomena which they were the first to investigate, and which have since been observed by many others, lend themselves readily to the explanation proposed by Laue, who supposed that electromagnetic waves of very short wave-lengths were diffracted by a set of small obstacles arranged on a regular point system in space. In analysing the interference pattern obtained with a zincblende crystal, Laue, in his original memoir, came to the conclusion that the primary radiation possessed a spectrum consisting of narrow bands, in fact, that it was composed of a series of six or seven approximately homogeneous wave trains.

In a recent paper† I tried to show that the need for assuming this complexity was avoided by the adoption of a point system for the cubic crystal of zincblende which differed from the system considered by Laue. I supposed the diffracting centres to be arranged in a simple cubic space lattice, the element of the pattern being a cube with a point at each corner, and one at the centre of each cube face. A simpler conception of the radiation then became possible. It might be looked on as continuous over a wide range of wave-lengths, or as a series of independent pulses, and there was no longer any need to assume the existence of lines or narrow bands in its spectrum.

* W. Friedrich, P. Knipping, and M. Laue, 'Münch. Ber.,' June, 1912.

† 'Camb. Phil. Soc. Proc.,' November, 1912.

Crystals as Indicated by their Diffraction of X-rays. 249

It is the object of this paper to extend the analysis used in the case of the zincblende to some other crystals, particularly those of the simple alkaline halides.

In treating the diffraction of waves by a space point system such as a crystal, that case is the most simple in which the diffraction is caused by a series of points arranged in a space lattice, of one of the 14 Bravais types. Here every point is identical with every other point of the arrangement, and it is always possible to find an element of the pattern consisting of a parallelepiped with a point at each corner: there will then be as many parallelepipeds as atoms in any space. The points can be referred to three axes parallel to the edges of the parallelepiped, and if one of the points is taken as the origin the co-ordinates of the others may be written

$$x = \pm pa, \quad y = \pm qb, \quad z = \pm rc,$$

where p , q , r are any integers, and a , b , c are equal to the sides of the parallelepiped, and therefore proportional to the axial ratios of the space lattice. When the axes are chosen in this way the co-ordinates of the points and the equations of the planes passing through given selections of points are expressed in the simplest manner possible.

Let a series of pulses fall on this space lattice, the direction of propagation having a given relation to the axes of the system. As any one pulse passes over each point, a diffracted wavelet spreads from it, and it will be shown that the wavelets from all the points due to one incident pulse will combine in certain directions to form trains of waves, which give rise to the patterns of spots appearing in Laue's diffraction patterns. This may be done in the following way:—

If the axial ratios of the space lattice be denoted by a , b , c , any plane which makes intercepts pa , qb , rc , on the axis (p , q , r being any integers) is parallel to a whole set of planes on which the points of the system may be considered as arranged. It is such planes as these which form the faces of a crystal. When a pulse falls on a set of points on a plane the wavelets from the points combine to build up a wave front which will appear to be regularly reflected from the plane. As there are a series of planes regularly spaced one behind the other, a single pulse falling on them gives rise to a reflected wave train.

When therefore a narrow pencil of X-rays falls on a section of a crystal, part of its energy is transmitted undeviated, but there is also a part which is reflected on the crystal planes existing potentially in the body of the crystal. It is the series of narrow beams arising by reflection in this way which gives rise to the pattern of spots appearing in the photograph.

There can be assigned to each set of parallel planes integral indices (h, k, l) , as when naming the faces of a crystal, and a spot can be classified as being reflected in the (h, k, l) set of planes. Here the integers h, k, l , are reciprocal to the intercepts which a parallel plane makes on the axis of reference. They are Millerian indices, the equation of the plane being

$$h\frac{x}{a} + k\frac{y}{b} + l\frac{z}{c} = \text{an integer.}$$

They may be considered as the parameters of each spot of the pattern, and are exactly equivalent to the parameters (h_1, h_2, h_3) employed by Laue in his original treatment of the subject. Laue defines his parameters by saying that the diffracted wavelet from a point at the origin of co-ordinates lags h_1, h_2, h_3 , wave-lengths in the directions under consideration behind the wavelets proceeding from its neighbours along the x, y, z axes respectively. Thus the wavelets from all atoms in the plane

$$h_1\frac{x}{a} + h_2\frac{y}{b} + h_3\frac{z}{c} = 0$$

are in phase with that from the origin, and, in general, the wavelets from all points in the plane

$$h_1\frac{x}{a} + h_2\frac{y}{b} + h_3\frac{z}{c} = \text{an integer}$$

are in the same phase. We are led back to the same conclusion as before, that the direction of the diffracted wave front is one in which the primary beam is reflected by planes whose Millerian indices are (h_1, h_2, h_3) . But, as will appear presently, it is important to bear in mind the fact that crystal structure alone fixes the exact position of the interference maxima, quite independently of the existence of homogeneous components of definite wave-length in the incident rays, and therefore a method of treatment has been adopted in which all reference to the wave-length has been avoided.

It is possible for a spot to appear in a position corresponding to reflection in any set of planes having integral indices (h, k, l) . In an actual pattern obtained by allowing the diffracted X-rays to fall on a photographic plate, since there is not an infinite number of spots, only a selection of the planes can be operative. The spots forming the pattern are of very different intensities, and one can never say that spots are entirely absent but merely that in certain cases the rays are too weak to make an impression. It would seem, however, that by classification of the planes which reflect the principal spots of the pattern a clue can be got to the true point system arrangement of the diffracting centres. The point system which affords the most simple interpretation of the pattern is that which ought to be taken as representing the crystal structure.

Crystals as Indicated by their Diffraction of X-rays. 251

When a photograph has been taken with a crystal an analysis is necessary in order to assign to each spot of the pattern obtained the correct parameters h, k, l , the Millerian indices of the face from which the spot is reflected. Having decided on the axes of reference of the crystal, the following method will be found to apply whatever their inclinations to each other and axial ratios may be.

The more important planes of the system are those densely packed with points, and from this fact it follows that these planes contain rows along which the points are closely packed. These are the important "point-rows" of the crystal, and each of these point-rows will have a set of important planes parallel to it. The three axes themselves are the most obvious examples of these point-rows. The "zone axis" of planes belonging to a common zone is also such a direction. There is a convenient relation between the points which are reflected in the planes belonging to any one zone. The reflected beam always lies on a circular cone with apex at the crystal section, the zone axis as axis, and the direction of the primary beam as one generator. This cone cuts the photographic plate in an ellipse passing through the central point of the pattern, and all spots reflected in planes of the zone lie on it. The arrangement of the spots on ellipses is very obvious in an interference pattern (see fig. 11), and the ellipses can immediately be drawn. A little calculation shows to which zone axis each ellipse must be assigned, and, by marking a given spot as lying on the intersection of two ellipses, the calculation of the indices h, k, l , of that spot is made possible. For each zone of planes we have the relation $hU + kV + lW = 0$ where (U, V, W) is the zone symbol; that is to say, the set of direction ratios of the zone axis.

When representing diagrammatically an interference pattern it is very inconvenient to draw the ellipses at the intersections of which the spots of the pattern lie. It is simpler to employ an extension of the usual stereographic projection of crystallography. Reference to fig. 1 will make this clear. Let the section of crystal be situated at C, the centre of the sphere represented in the figure by the circle ABP, and let the direction of the incident rays be from P to C. The rays which traverse the crystal undeviated fall on the photographic plate AD at A. Let CZ represent the direction of a zone axis. The beams reflected in planes of this zone lie on a circular cone with vertex at C, of which CZ is the axis, and CA, CB are two generators.

This cone cuts the sphere in a circle of which AB is a diameter, and by the well known property of the stereographic projection, the projection of this circle on the plane AD from the pole P is also a circle. The centre of this circle is at Z, since $AZ = ZS'$, Z being the point where the zone axis cuts the photographic plate.

Let the pattern of spots be supposed to be made by the diffracted beams on the sphere ABP , and this pattern projected on the plane AD from the pole P . Spots corresponding to reflection in planes of a zone now lie on a circle, having its centre at the point where the zone axis cuts the plate AD . The spot at S made by the reflected beam CB becomes a spot at S' of the

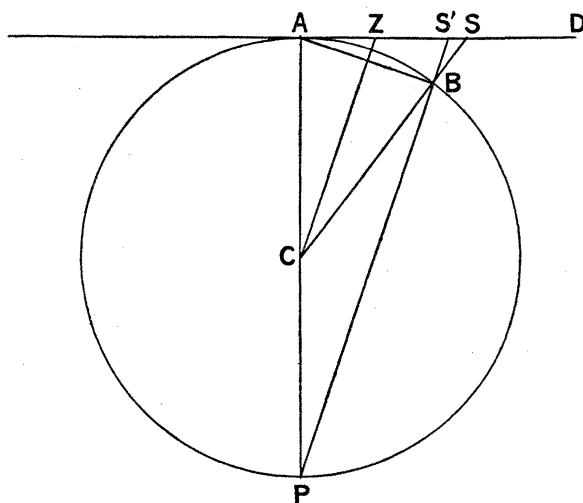


FIG. 1.

transformed pattern. The distortion of the pattern of spots by the transformation is very small except in the regions distant from the centre, and circles are much easier to draw than ellipses. This has been done in all the diagrams given in this paper. In constructing a diagram, a point is chosen as that in which the incident rays meet the photographic plate. This is A in the figure. Then the points such as Z , where the principal zone axes meet the plate, are found by a calculation, which is easy when the crystal is placed symmetrically to the pencil of X -rays. A circle is drawn with centre Z and radius ZA . This being done for each zone axis, the intersections of the circles give the stereographic projections of the reflected spots.

Let us take as an example of the application of this analysis the very simple case of potassium chloride. The diffraction pattern obtained when the X -rays fall normally on a plate cut parallel to the cube face (001) is reproduced in fig. 2, Plate 10, and its stereographic projection in fig. 3, which shows also the indices of the reflecting planes corresponding to the several points of the photograph.

Potassium chloride is cubic, and the indices given to the planes are those obtained when the edges of the cube are selected as axes of reference.

Crystals as Indicated by their Diffraction of X-rays. 253

The circles correspond to zone axes for which

$$\left. \begin{array}{l} U = 0, \quad V = \pm 1 \\ U = \pm 1 \quad V = 0 \end{array} \right\} W = 0, 1, 2, 3, 4, 5,$$

and their intersections give the spots reflected in all planes of the form $(h k l)$ where h and k have any of the values

$$0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5.$$

In the diagram of the KCl pattern the spots are represented by dots, the magnitude of each dot indicating the strength of the corresponding spot in the

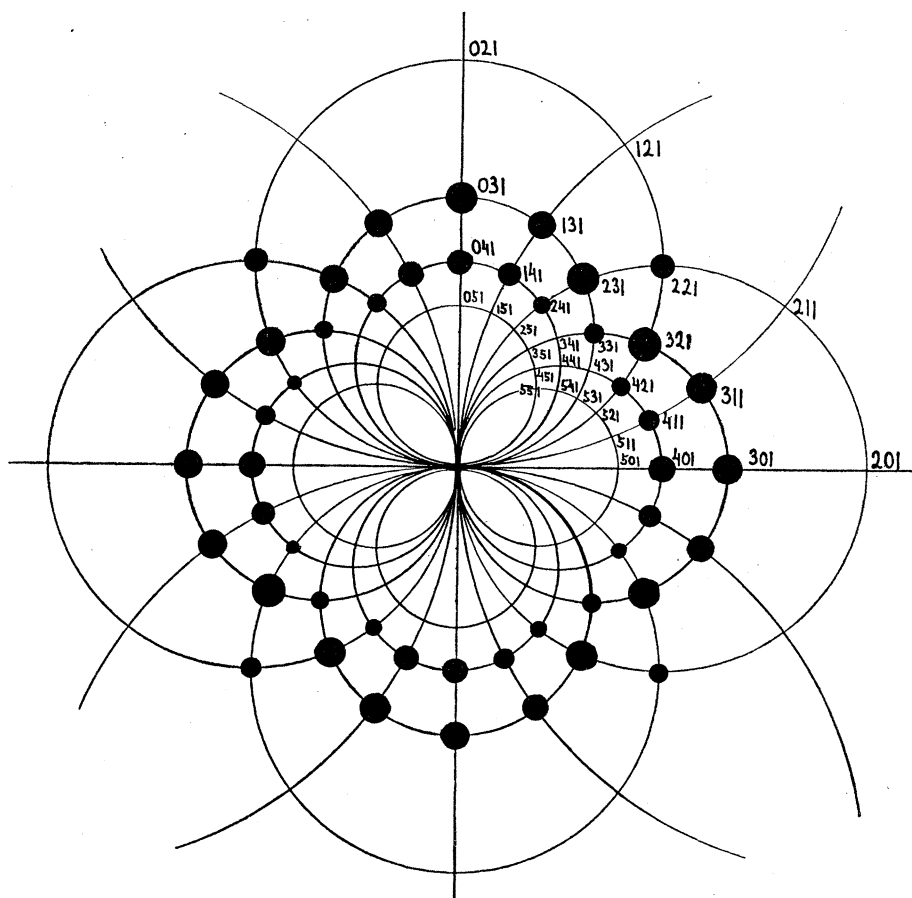


FIG. 3.—Potassium chloride.

photograph. It will be seen how complete the pattern is, and how within a certain range each intersection is represented by a spot in the photograph.

This may be put in another way. Below is a table of values of h and k , l being equal to 1. In the square corresponding to given values of h and k

is placed a dot denoting the magnitude of the corresponding spot, the square being left empty if no spot is to be seen.

Table I.

KCl.

		$h \rightarrow$					
		0	1	2	3	4	5
$k \downarrow$	0				*	*	
	1				*	*	
	2			*	*	+	
	3	*	*	*	+		
	4	*	*	+			
	5						

This table contains a list of all the spots appearing in the photograph. It suggests that the diffraction is due to a simple cubic space lattice, for when the elementary parallelepiped is a cube and its edges are taken as axes the indices of the planes naturally take these simple forms.

For, let a series of planes be taken, for which two indices are constant and one varies, such as the series 031, 131, 231, 331, 431, etc. These planes will be arranged in this order for all their properties, such as reticular density, distance apart, and so forth, if, and only if, the indices are referred to axes parallel to the sides of the elementary parallelepiped. If this condition is satisfied, then all the properties of the planes vary in an orderly manner as one passes along the series. The power of reflecting the X-rays is a particular property of the planes, which is seen from the photograph to vary continuously for any such series as the one given above, therefore the diffracting system is a space lattice with axes at right angles, and a cube for its elementary parallelepiped.

It may be objected here, that it is conceivable that a complex structure, and a radiation consisting of homogeneous components, just happen in the case of potassium chloride to give a deceptively simple pattern. That this is not the case can be seen by displacing the crystal from its symmetrical position, and obtaining the distorted interference pattern. It is still as straightforward as before, though of course no longer symmetrical. Corresponding spots in the two patterns are now made by different wave-lengths, and it is obvious that there can be nothing of the nature of homogeneous components of the incident radiation. The contrast of this pattern with those characteristic of potassium bromide and iodide, of rock salt, and of zincblende, which will shortly be given, will tend to make this more clear.

Crystals as Indicated by their Diffraction of X-rays. 255

All the most intense spots of the photograph are at about the same distance from the centre of the pattern. A circle can be drawn such that the spots which lie near to it are very intense, while those further away are weaker and those at great distances are too faint to appear. All ellipse intersections lying near this circle are represented by a spot. Those planes reflect most strongly for which the glancing angle lies between 12° and 20° and it is in seeking to explain this fact that it is necessary to consider the question of the "wave-length" of the diffracted rays. This we must now do.

When a pulse falls on a series of planes regularly spaced one behind the other, it is reflected as a wave train, and the waves making any one spot must be considered to be of the lengths given by

$$n\lambda = 2d \sin \theta,$$

where θ = glancing angle, d = distance between successive planes, and n is an integer 1, 2, 3, etc. An alternative way of regarding the phenomenon is to consider the incident radiations as compounded of homogeneous wave trains of all wave-lengths, with a characteristic distribution of energy in the spectrum, when the parallel planes must be considered as reflecting only that part of the spectrum for which the relation $n\lambda = 2d \sin \theta$ holds good. In the case of the cubic space lattice considered here, this relation reduces to

$$n\lambda = \frac{2a}{l} \sin^2 \theta,$$

where a is the distance between neighbouring points along the cubic axes, for a simple calculation shows that $d = a \sin \theta / l$. Since l is equal to unity for all the spots of the potassium chloride photograph, spots which have the same θ , and lie at the same distance from the centre of the pattern, correspond to the same wave-length. The ring of intense spots in the pattern indicates strong reflection of a certain part of the spectrum of the incident radiation. Either conditions are especially good* for reflecting this wave-length, or the incident rays have a large amount of their energy in this part of the spectrum.

It is interesting to compare the simple pattern of potassium chloride with those of potassium iodide, potassium bromide, fluorspar, and zincblende.

The stereographic projection of KBr (100) is given in fig. 4, that of KI being very similar. Both of these are like the patterns of zincblende and fluorspar, and are in marked contrast to that of KCl.

* The most important condition in this connection is probably the thickness of the crystal section used. As will be shown later, the use of a thin crystal section favours the reflection of the longer wave-lengths, the corresponding spots coming out strongly, while the use of a thick section favours the reflection of the shorter.

It is evident that some factor has now entered which destroys the simplicity of the arrangement of spots characteristic of potassium chloride. Spots no longer appear at every intersection of the ellipses within a certain region, as

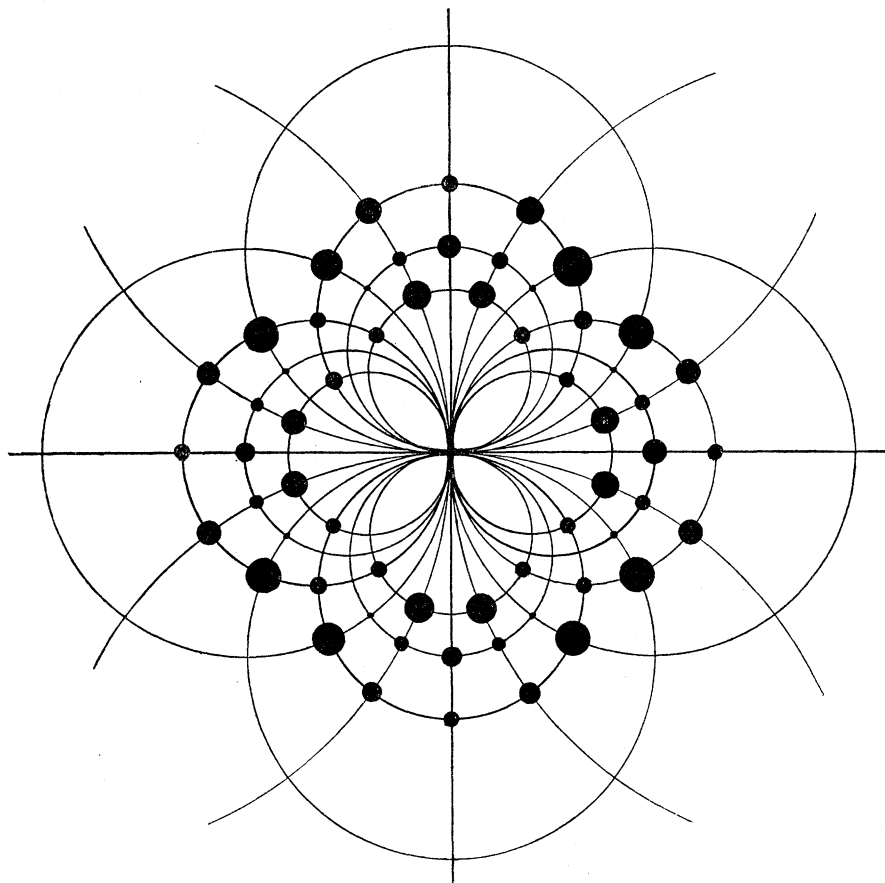


FIG. 4.—Potassium bromide.

in fig. 3. A tabulation of the intensities of the spots in the zincblende and potassium bromide patterns will make this clear. (See Tables II and III.)

There are also in the case of zincblende several spots for which a value 3 must be assigned to l , if h and k are to be integers, but not many. It was a consideration of Table II which led in a former paper* to the conclusion that the diffracting centres of the zincblende crystal are arranged on the face-centred cubic space lattice.

An examination of the planes in which reflection takes place shows that there is a differentiation between those whose indices are wholly odd and

* 'Camb. Phil. Soc. Proc.,' November, 1912.

Crystals as Indicated by their Diffraction of X-rays. 257

Table II.

		Zn.S.							
		$h \rightarrow$							
$h \downarrow$	h	0	1	2	3	4	5	6	7
	0				+				
	1			•	+	*	*		+
	2		•	•	*	+			
	3	+	+	*	+	+	*		+
	4		*	+	+				
	5		*		*		+		
	6								
	7		+		+				

Table III.

		K.Br.					
		$h \rightarrow$					
$h \downarrow$	h	0	1	2	3	4	5
	0				+	*	
	1				*	+	*
	2				*		
	3	+	*	*	+		*
	4	*	+				
	5		*		*		
	6						
	7						

those which have one or more even indices. If those planes alone are considered which have odd indices, as in the following table, the scheme is as complete as it was for the spots of the KCl crystal.

Table IV.

		Zn.S. (odd indices only)				
		$h \rightarrow$				
$h \downarrow$	h	1	3	5	7	9
	1		+	*	+	
	3	+	*	*	•	
	5	*	*	+		
	7	+	•			
	9					

Odd planes, ZnS.

Table V.

		Zn.S. (even indices) only					
		$h \rightarrow$					
$h \downarrow$	h	0	1	2	3	4	5
	0				+		
	1			•		*	
	2		•	+	*	•	
	3	+		*		•	
	4		*	•	•		
	5						

Even planes, ZnS.

The same is true for those with an even index* except that the intense spots are all further removed from the centre of the picture.

This difference can be explained without our being forced to assume that the diffracting system is anything more than a simple system of identical points. It is sufficient to suppose that the point system has points at the centres of the cube faces as well as at the cube corners. Let a cubic point system of the first kind be taken which has points at cube corners alone, and let points be introduced at the cube face centres in order to turn it into a

* The spot 041 forms an exception, indeed evidence is not lacking that the assumption of diffraction by the face-centred space lattice does not completely account for the pattern. The reason for this will appear when the parts played by the atoms of two kinds in the diffraction are discussed.

point system of the so-called "third kind." (The "second kind" is the centred cube.) The spacing of the planes which have odd indices (h, k, l) is not altered by the introduction of the new points, for they all lie on the original planes and only increase their point density. On the other hand, in the case of planes having an even index, some of the new points lie half-way between the original planes, the distance between the successive planes of this type must now be halved, and so must therefore the wave-lengths of the reflected beams.

The interpretation of the zincblende pattern is now simple. We have seen that the planes with odd indices only are a complete set. There are fewer spots corresponding to reflection in planes with an even index, for these planes are, relatively to the former, less closely packed, and of a more complex nature. Moreover, they are, at the same time, less widely separated, and therefore the intense spots with even indices are further from the centre; the angle of incidence must be increased in order to make these planes reflect that region of the spectrum which gives intense spots. By assuming the third cubic space lattice instead of the first, all the intense spots of the pattern again correspond to the same wave-length region.

The difference between the diffraction by the two cubic space lattices may be put in a much clearer way on analysis of the patterns of threefold symmetry, obtained when the incident rays fall normally on a plate cut perpendicular to a trigonal axis. If the points of the space lattices are considered from this aspect, they are special cases of the trigonal rhombohedral space lattice, one of the Bravais types.

The axes to which the spots ought to be referred are not the same for the two cubic lattices. When the points are at cube corners alone, the axes along which they are nearest neighbours are the cube edges, and the cube itself is the elementary parallelepiped. When there are also points at the centres of the cube faces, three semi-diagonals of cube faces meeting in a corner form three edges of the elementary parallelepiped. The angles between the axes are right angles in the first case, in the second they are 60° .

It will now be clear that when the stereographic diagram is constructed, giving the positions of the spots reflected from the simple planes of a trigonal rhombohedral space lattice, one such diagram will represent the patterns of all rhombohedral lattices, the alteration of the angle between the axes, *i.e.*, the rhombohedral angle, only causing an alteration of the scale of the diagram. The radius of the sphere used in the projection is, of course, supposed to be always the same.

Given the points where the three axes of the lattice meet the diagram, the corresponding points for the other zone axes can immediately be found and

Crystals as Indicated by their Diffraction of X-rays. 259

the whole diagram drawn. Such a diagram is shown in fig. 5, X, Y, Z, being these axial points, Now, our study of the patterns of fourfold symmetry given by potassium chloride and zinblende has shown that the axes of the

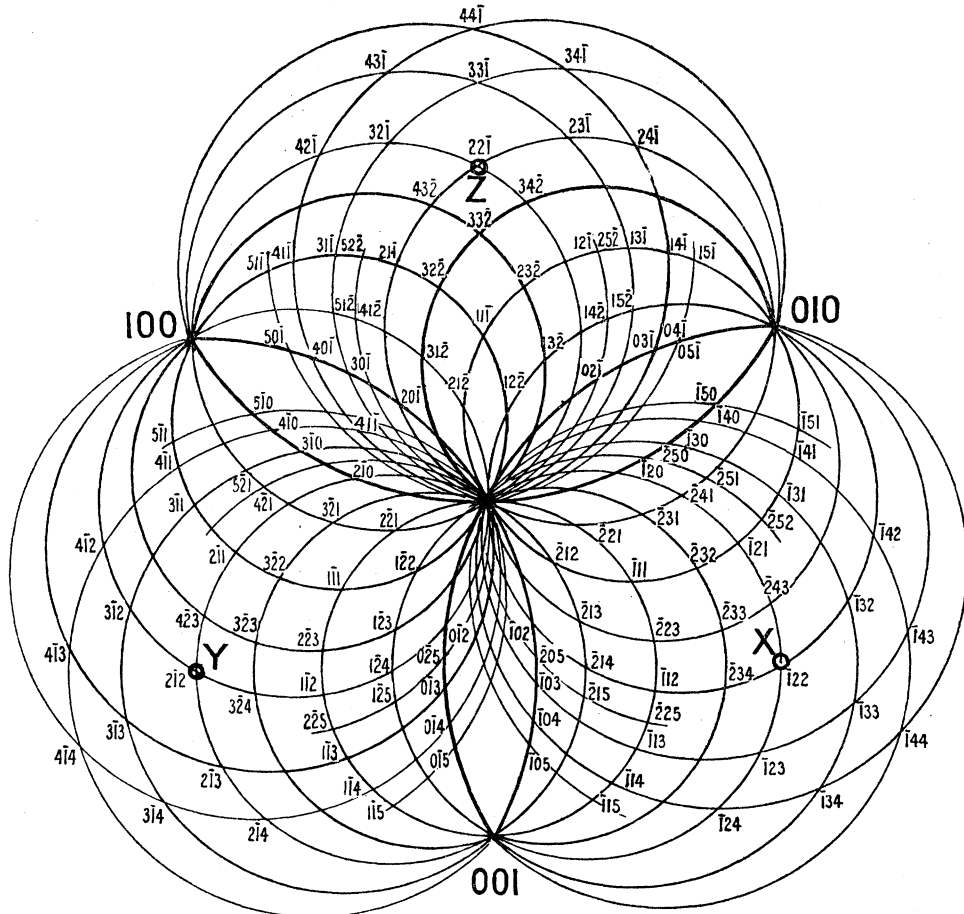


FIG. 5.

lattice, which is from this aspect a special case of the rhombohedral lattice, make angles of 90° with each other in the first case, and of 60° in the second. Therefore it ought to be possible to refer the threefold patterns of potassium chloride and zinblende to the same trigonal lattice diagram, the scale being different, however, in the two cases. This conclusion is exactly confirmed by experiment. The pattern given by zinblende was published by Laue in his original memoir. The stereographic projections of the zinblende and potassium chloride patterns are given in figs. 6 and 7. The object of this comparison is to show that the spots of the KCl pattern fall naturally on

a diagram twice the size of that on which the spots of the ZnS pattern are arranged, the points where the axes making 90° with each other cut the plate, being just twice as far apart as for axes making 60° with each other.

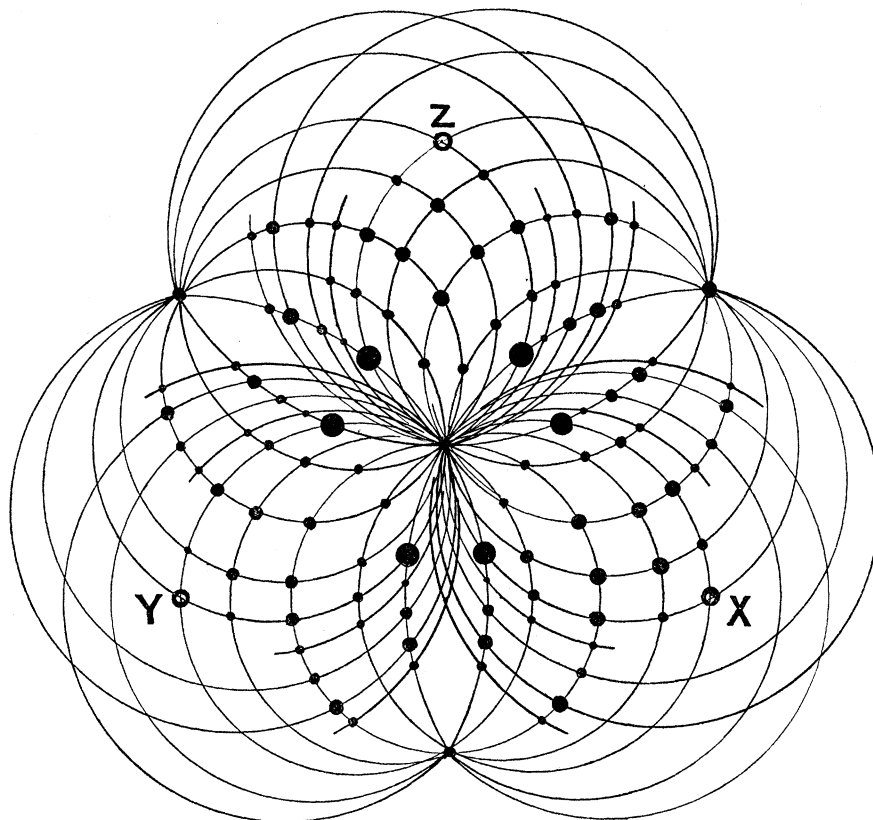


FIG. 6.—Zincblende.

The following table will illustrate the awkwardness of referring either pattern to the wrong diagram.

If the spots of the zincblende pattern are referred to the cubic axes, their indices become very much more complicated, and the pattern is no longer complete. The converse is true for the potassium chloride pattern, the indices in this case being simpler when referred to cubic axes. In Table VI a list of indices of the spots of each pattern is set down referred to (A) the cube edges, (B) the cube face diagonals, *i.e.*, three edges of the regular tetrahedron, as axes.

It will be seen that in the case of zincblende it is the B series, in the case of the potassium chloride the A series, which is simple, and which gives a complete series of indices over a certain range. I do not think there can be any doubt which space lattice is the right one in either case.

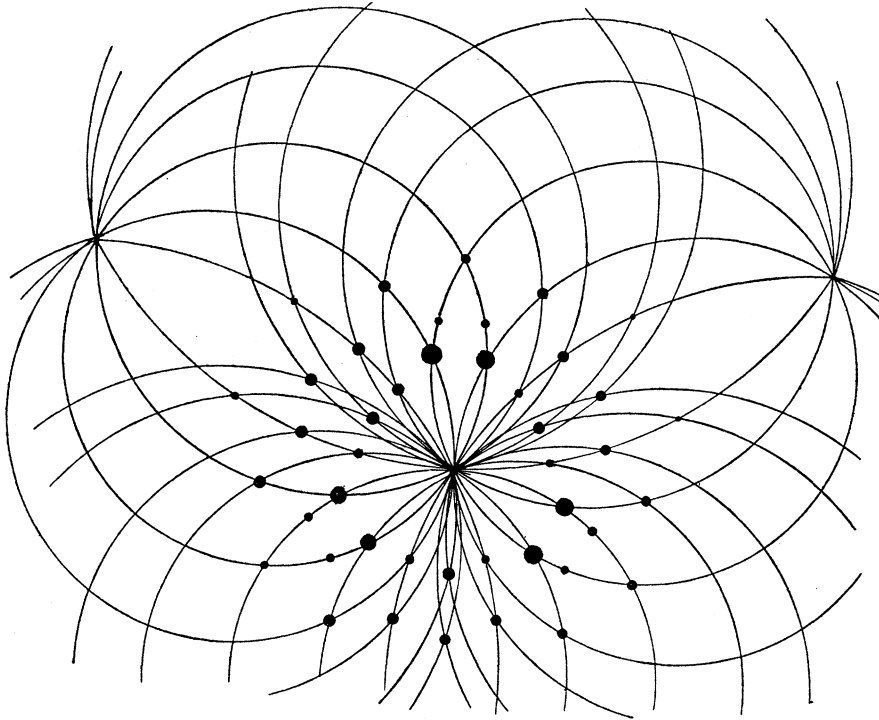
Crystals as Indicated by their Diffraction of X-rays. 261

Fig. 7.—Potassium chloride.

Table VI.

Zineblende.				Potassium chloride.*	
A.	B.	A.	B.	A.	B.
$\bar{1}11$	010	$\bar{1}11$	100	$3\bar{1}\bar{1}$	$11\bar{1}$
$3\bar{3}2$	0 $\bar{5}1$	$3\bar{7}5$	$51\bar{1}$	$20\bar{1}$	$21\bar{1}$
$5\bar{5}3$	0 $\bar{4}1$	$\bar{1}32$	$41\bar{1}$	$31\bar{2}$	$41\bar{1}$
221	031	$\bar{1}53$	$31\bar{1}$	$11\bar{1}$	100
$3\bar{3}1$	0 $\bar{2}1$	$\bar{1}95$	$52\bar{2}$	$30\bar{2}$	$31\bar{2}$
$\bar{1}10$	0 $\bar{1}1$	0 $\bar{2}1$	$21\bar{1}$	$21\bar{2}$	$30\bar{1}$
		173	$32\bar{2}$	$41\bar{1}$	$33\bar{2}$
		$\bar{1}31$	$11\bar{1}$	$32\bar{3}$	$50\bar{1}$
		$3\bar{5}1$	$12\bar{2}$		

* The indices of the A series for the KCl pattern may not, at first sight, appear simpler than those for the B series. The B series, however, is curiously incomplete. For instance, $21\bar{1}$ and $41\bar{1}$ occur but no $31\bar{1}$; $50\bar{1}$ and $30\bar{1}$ but no $40\bar{1}$; $33\bar{2}$ and $31\bar{2}$ but no $32\bar{2}$. In fact, there is a tendency for the sum of the indices to be even, and such a selection of the simple planes as this always implies that the wrong axes have been taken.

In the B list for ZnS, indices such as $(52\bar{2})$ are intermediate between $31\bar{1}$ and $21\bar{1}$.

In the case of rock-salt, it is not possible to regard the pattern as completely characteristic of the one point system or the other. Photographs obtained using a thin section of crystal, about 1 mm. thick, cut parallel to a cube face, show a pattern very similar to that given by potassium chloride, though in no case are they so simple as the pattern given by the latter crystal; for a considerable amount of difference between the "odd"

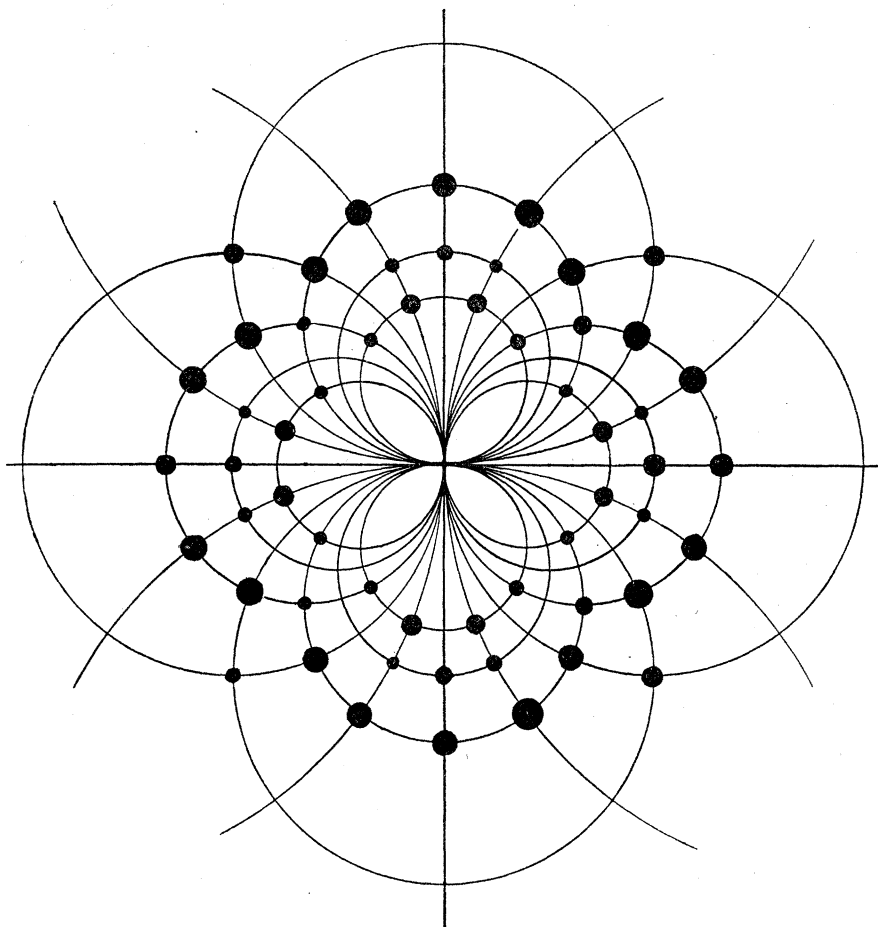


FIG. 9.—Rock-salt, 2.5 mm. thick.

and "even" planes is also evident. A photograph taken with a section 6 mm. in thickness is more like one taken with potassium bromide or iodide, the difference between odd and even planes being more marked. In fig. 8, Plate 10, is reproduced a photograph taken with a section of rock-salt, 2.5 mm. thick, cut parallel to a face (100), and in fig. 9 its stereographic diagram. In the tables on the next page are set down the intensities of the spots when different thicknesses of crystal are used.

Crystals as Indicated by their Diffraction of X-rays. 263

Table VII.

$h \rightarrow$	1 mm.					
	0	1	2	3	4	5
0				*	+	
1			•	*	+	+
2		•	*	*		
3	*	*	*	*		+
4	+	+				
5		+		+		

NaCl, 1 mm.

Table VIII.

$h \rightarrow$	2.5 mm.					
	0	1	2	3	4	5
0				+	+	
1				*	+	*
2			•	*		
3	+	*	*	+		+
4	+	+				
5		*		+		

NaCl, 2.5 mm.

Table IX.

$h \rightarrow$	6 mm.					
	0	1	2	3	4	5
0					+	
1				+	+	*
2				*		
3		+	*	+		+
4	+	+				
5		*		+		

NaCl, 6 mm.

I think these tables, especially the first one, suggest that the rock-salt diffracting system is in some way intermediate between those of potassium chloride and potassium bromide. The change of intensity of the spots with the thickness of the crystal is interesting. It may be laid down as a general rule that increasing the crystal thickness increases the intensity of the inner spots as compared with that of the other. This is to be expected, for the inner spots represent the shorter and more penetrating radiations.

If in passing through a thickness dx of the crystal a proportion αdx of the radiation of a certain wave-length is reflected, and if the absorption coefficient of the radiation in the crystal is k , then the radiation reflected in a slip of crystal of thickness t will be proportional to $\alpha t e^{-kt}$ to a rough approximation. This is a maximum when $t = 1/k$, and since α is very small, this means that to get a spot strongly marked a section of crystal should be used of such thickness that it absorbs a fraction $1/e$ of the incident radiation of that wave-length. This would explain qualitatively the variation with thickness of crystal of the intensity distribution over the spots which is actually observed.

On comparing the evidence as to the nature of the diffracting systems in these crystals of sodium chloride, and of potassium chloride, bromide, and iodide, it would seem that a very simple explanation of their curious difference may be arrived at when it is considered that in each case diffraction is caused by two different atoms, and that the relative efficiencies of the two vary from crystal to crystal. Any explanation of these differences would be an extremely improbable one which did not assume a similar structure for the whole group of alkaline halides, for these crystals resemble each other very closely in their properties. Yet it has been seen that the space lattice of diffracting points is the simple cubic one in KCl; it is the face-centred cubic lattice in KBr and KI, and that in the case of NaCl the

diffracting point system is in some way intermediate between the two space lattices.

Let us consider on what atomic properties the relative efficiencies might depend. It has been firmly established that the absorption of X-rays depends on the relative proportions of the various elements contained in the absorber. It is a purely additive property of the weight of each element per cubic centimetre of the absorber, and does not depend on the manner in which the elements are combined. Also the absorption of homogeneous X-rays increases steadily with the atomic weight of the absorber, except for a sudden discontinuity consisting of a large drop in the absorption coefficient when the atomic weight of the absorber passes through that of the element of which the homogeneous X-rays are the characteristic radiation. There are, however, no discontinuities in the absorption coefficient corresponding to the changes in chemical properties of the elements in the periodic table as one passes to higher atomic weights. It is reasonable, therefore, to assume provisionally that the weight of the atom in the main defines its effectiveness as a diffracting centre, and that two atoms of equal weight are equally effective. In the case of potassium chloride the atoms of potassium and chlorine, of atomic weight 39 and 35.5 respectively, are sufficiently close in atomic weight to act as identical diffracting centres. For rock salt this is no longer true; the atomic weight of sodium and chlorine differ considerably (35.5 to 23), and complications are introduced into the simple pattern characteristic of potassium chloride. In potassium bromide and iodide one atom preponderates so greatly over the other in atomic weight that the diffracting system consists practically of atoms of one kind only, and the pattern can again be assigned to a simple space lattice, but one which is of a different nature to that of potassium chloride. Yet the atoms of alkaline metal and halogen have precisely the same arrangement in all these cases.

Let us distinguish between two kinds of diffracting points by calling them black and white. Then the points must be arranged in such a way that—

1. There are equal numbers of black and white.
2. The arrangement of points black and white taken all together is that of the first cubic space lattice.
3. The arrangement of blacks alone or of whites alone is that of the third cubic space lattice.

An arrangement which gives this result is shown in fig. 10.

In this diagram we may associate black centres with the alkaline metal, and white with the halogen, or *vice versa*. The space lattice formed by the whites is the same as that formed by the blacks, being in each case the face-

Crystals as Indicated by their Diffraction of X-rays. 265

centred cube. If black and white centres become identical, as in potassium chloride, the diffracting lattice becomes the simple cubic one.

The evidence for this arrangement in the alkaline halides seems very strong, but this does not by any means complete the solution of their

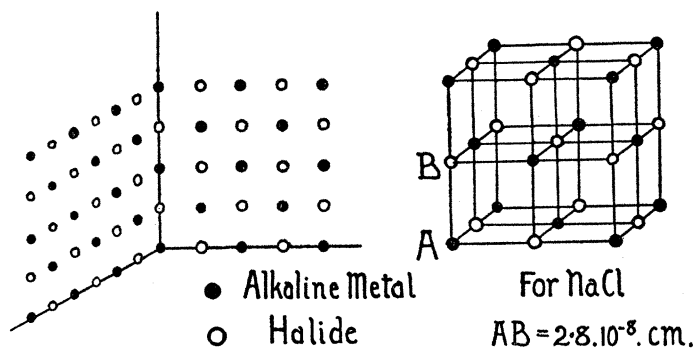


FIG. 10.

structure. It yet remains an open question whether one atom alone is to be associated with each point of the system, so that, for example, the black and white centres actually represent sodium and chlorine atoms in rock salt, or whether the crystal structure is of a more complex nature. It was with the object of discovering the complexity of the diffracting unit of these and other crystals that the series of crystal pattern analyses, which will now be described, were made; their results would seem to indicate clearly the association with each diffracting centre of a single atom.

It was shown above that the stereographic diagram, giving the position of spots reflected in the planes of a trigonal rhombohedral lattice, is the same except for scale for lattices of any rhombohedral angle. The completeness with which the spots of the zincblende pattern whose projection is given in fig. 6 represent the intersections of the circles of the diagram for the trigonal lattice would suggest that in all cases in which diffracting centres were arranged on a trigonal lattice, the pattern obtained would be very much the same. At all events, this would be so when the rhombohedral angle is not very different from 60° . That this is actually the case is well shown by the stereographic projections in figs. 12 and 13. They are the projections of photographs taken with sections of flourspar and calcite, cut perpendicular to a trigonal axis, the flourspar photograph being given in fig. 11, Plate 10. It is clear that in this case also, as in that of zincblende, every simple plane of the lattice reflects a spot when the angle of incidence lies within a certain range. Corresponding spots in the three diagrams vary very much in intensity, but this is to be expected. The point which it is desired to

make clear is the certainty with which the correct axes of the lattice may be found from a study of the pattern. In the case of fluorspar, as in that of zincblende, the rhombohedral angle of these axes is 60° . In the case of calcite it is slightly greater, a calculation of this angle and a comparison of the orientations of crystal and pattern making it clear that the axes of the lattice are three diagonals of rhombohedron faces meeting in an obtuse corner of the calcite rhombohedron, not the edges of the rhombohedron,

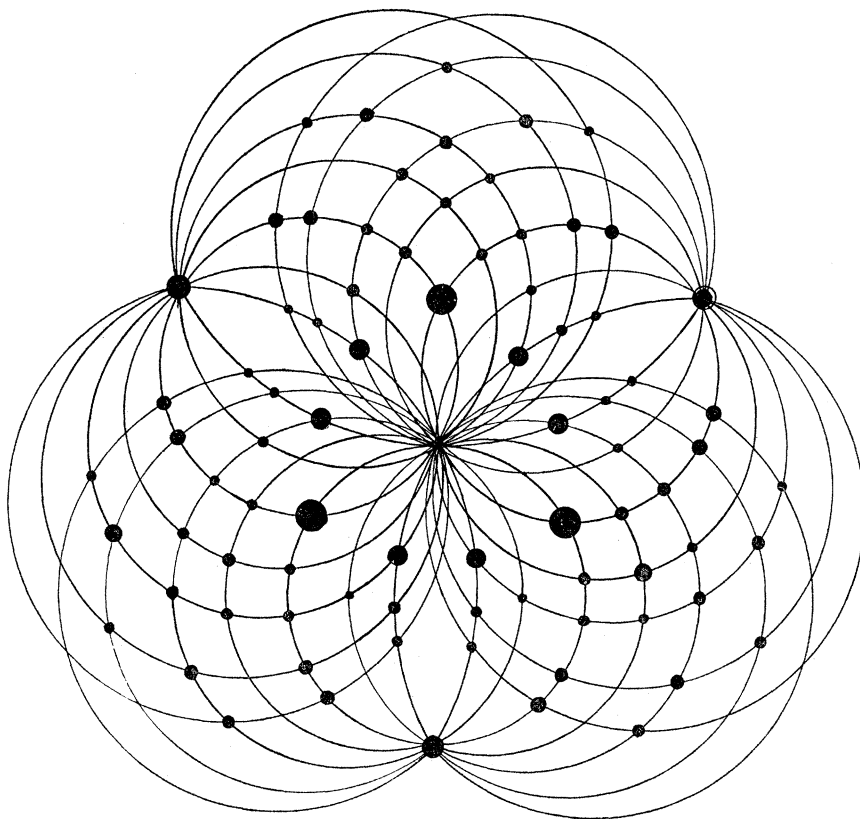


FIG. 12.—Fluorspar.

which are generally taken as the axes to which the faces of a calcite crystal are referred.

In these three cases, zincblende (ZnS), fluorspar (CaF_2) and calcite (CaCO_3), the diffracting centres are thus arranged on one space lattice. But, since a space lattice is an arrangement in which each point is related to its neighbours in exactly the same way as every other point, it would be impossible to arrange complex molecules in a space lattice unless only one point in each molecule is effective. It is difficult to avoid the conclusion

Crystals as Indicated by their Diffraction of X-rays. 267

that the molecule acts as a single point because it contains in each case one atom of much greater atomic weight than the others. A comparison with a case in which this is not so is afforded by the rock-salt pattern of threefold symmetry given in fig. 14 and Plate 10, fig. 15; it will be seen how awkwardly it fits the diagram. There is a certain want of symmetry in the figures, which must not be confused with the want of fit. Its pattern is, in fact, intermediate between that characteristic of axes of rhombohedral angle

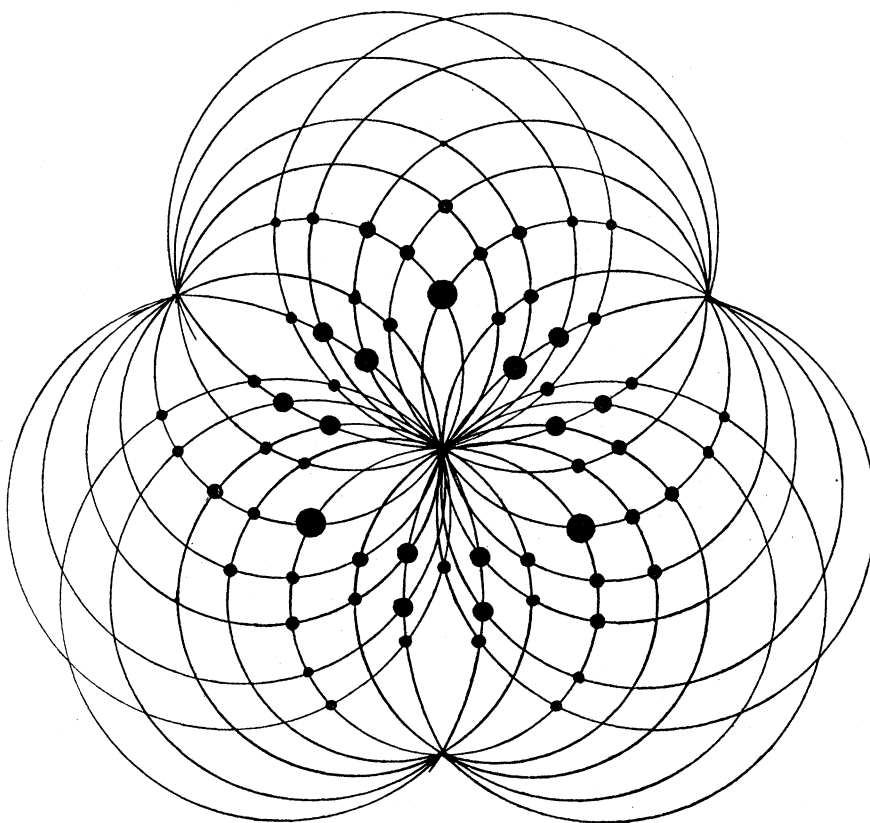


FIG. 13.—Calcite.

at 60° and that of axes at 90° , just as was the case with its pattern of fourfold symmetry.

Having found the nature of the simple diffracting lattice in these three cases and that of the alkaline halides, the final step in the argument which would assign a single heavy atom to each diffracting centre is made below by a comparison of the scale of their lattices, that is, a comparison of the length of the sides of the elementary parallelepiped for different crystals. Since the diffraction is caused by the heavy atoms, and there is only one in

each molecule, this conclusion, if correct, will mean an association of one molecule with each parallelepiped of the lattice.

In a paper to the Royal Society, read in April, 1913,* a method was described of analysing the radiations from an X-ray bulb by reflecting them from the face of a crystal, and measuring the ionisation produced by the reflected beam.

The apparatus devised for this purpose resembled a spectrometer; the

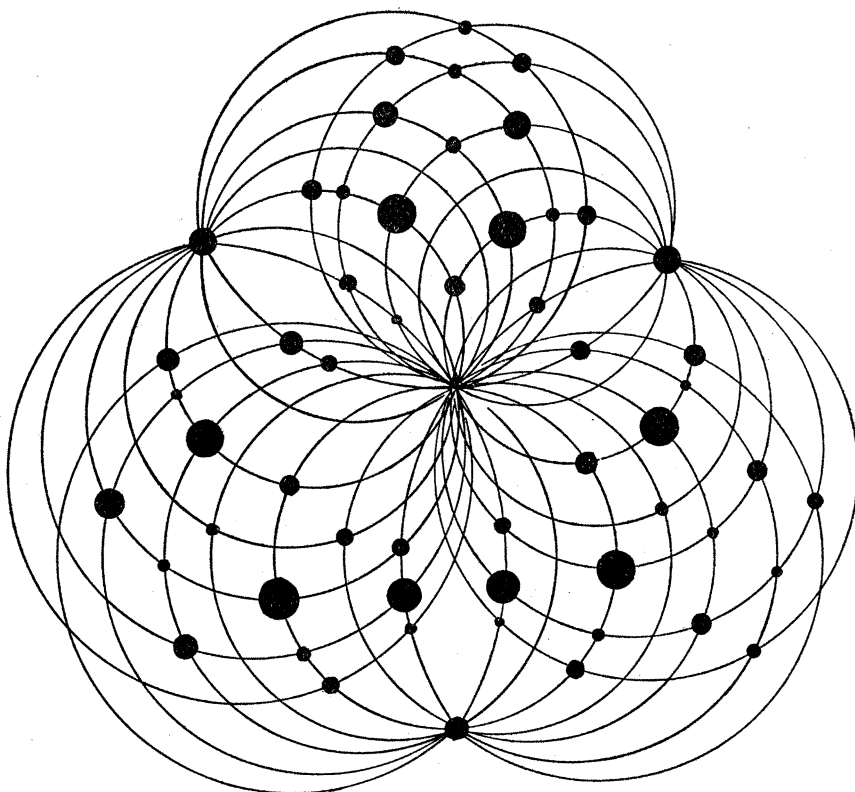


FIG. 14.—Rock-salt.

crystal was set on a revolving table at the centre of the instrument, and irradiated by a narrow beam of X-rays passing through a collimator slit. The reflected beam was received, and its ionisation measured, in a chamber mounted like the spectrometer telescope. By means of this instrument it was possible to measure the strength of the reflected beam when an approximately constant beam of rays fell on the face of the crystal at varying angles of incidence. The results of the measurement made with a crystal face may be summed up in a curve, in which the strength of the

* W. H. Bragg and W. L. Bragg, 'Roy. Soc. Proc.' July 1, 1913.

Crystals as Indicated by their Diffraction of X-rays. 269

reflected beam is plotted against the glancing angle at which the rays fell on the crystal. With most crystals, such a curve shows that at all angles there is a general reflection of the rays, the reflection being much stronger at the more glancing angles. Superimposed on this, as it were, there is at certain very sharply defined angles a special reflection of very great intensity as compared with the general reflection. This special reflection shows itself as very marked peaks on the curve, the amount of ionisation in the chamber becoming perhaps 20 times as great as the chamber is swept through the region of a peak, and then falling away to its normal value again, the whole taking place within settings a degree apart.

The results which we obtained with various crystals pointed to the existence of at least three components of the X-ray beam of definite wavelength, reflected from a crystal face when the condition

$$n\lambda = 2d \sin \theta$$

is satisfied for the component and crystal in question. Here λ is the wavelength, θ the glancing angle, and d the distance between successive planes of the crystal structure parallel to the reflecting face. The number n represents the "order" of the reflection, for several peaks, which can be recognised as belonging to the same homogeneous radiation by the identity of their absorption coefficients, appear at a series of angles whose sines are in the ratio 1 : 2 : 3.

It will possibly be objected here, that in the previous discussion of the interference patterns, the spectrum of the incident radiation has been taken to be continuous, the simplicity of the potassium chloride photograph supporting the view; while here direct evidence of the existence of homogeneous components of the radiation has been obtained. This difficulty disappears when the wave-lengths to be assigned to the spots of the interference pattern, and to the peaks of the curve, are compared. For instance, in the potassium chloride pattern of fourfold symmetry (fig. 2) the spot formed by the longest waves is reflected in the planes (221), and if a is the side of the elementary cube of the lattice of this crystal, the wave-length to be associated with the spot, from the formula

$$\lambda = 2d \sin \theta = 2a \sin^2 \theta$$

is equal to $a \times 0.22$. On the other hand, the peak corresponding to the homogeneous radiation of shortest wave-length is reflected from the face (100) of the same crystal at an angle of about 8.4° , and corresponds to a wave-length $a \times 0.29$ nearly. The spots of the pattern thus correspond to a region of the spectrum well inside the peaks on the reflection curve, and, in general, this is true for all the patterns. The reflection curve, indeed, bears

out well the assumptions as to the continuous nature of the spectrum of the radiation giving the spots, for at all angles less than 10° a strong reflection takes place which only falls away slowly as the glancing angle is increased. The very fact that in most photographs the incident rays are parallel to an axis of symmetry ensures that no important planes occur making such an angle with the primary rays as to reflect the homogeneous components.

It is possible to recognise the same three peaks, which will be referred to as A, B, C, in the curves drawn for reflection in the faces of almost all crystals which have been tried. They are always of approximately the same relative height, they have each a characteristic absorption coefficient, and they are spaced in the same way on the curves. There appears to be no doubt that three lines* exist in the spectrum of the incident radiation, which give rise to the peaks. This being so, one has a means of finding with some accuracy the ratio of the values of d , the distance between successive planes of the structure, for different crystals and different faces of the same crystal.

The angles at which these peaks are reflected from the various faces of a crystal, and from faces of different crystals, thus afford a great insight into the crystal structure; and, in fact, they supply just that information concerning the structure which the interference patterns do not, for by their means the dimensions of the lattices of different crystals can be accurately compared. The interference patterns only supply information concerning the nature of the lattices.

An analysis of the results obtained when different faces of the same crystal are used to reflect the X-rays in the spectrometer will show how this comparison is carried out.

In the curves for reflection from the three primary planes of the rock-salt crystal (100), (110), (111), (two of which are shown in fig. 16), the peaks occur for each face, but at different angles. From the equation

$$\lambda = 2d \sin \theta,$$

θ being the angle for the peak of the first order in each case, we have, for these three faces

$$d_{(100)} : d_{(110)} : d_{(111)} :: \frac{1}{\sin \theta_{(100)}} : \frac{1}{\sin \theta_{(110)}} : \frac{1}{\sin \theta_{(111)}},$$

where $d_{(100)}$ is the distance between planes parallel to the face (100), $\theta_{(100)}$ the angle at which the most prominent peak is reflected from the same face.

* By using narrow slits in the reflection apparatus, evidence of the existence of more than three lines has been obtained, the B and C peaks being really double. See fig. 16.

Crystals as Indicated by their Diffraction of X-rays. 271

The angles for these three faces are 11.4° , 16.0° , 9.8° , respectively. This gives the result

$$d_{(100)} : d_{(110)} : d_{(111)} :: 1 : 0.718 : 1.16,$$

whereas
$$1 : \frac{1}{\sqrt{2}} : \frac{2}{\sqrt{3}} :: 1 : 0.707 : 1.15,$$

these being the theoretical relations for the face-centred cubic space lattice. This does not comprise all the information which a study of these three curves yields, they will be analysed more carefully below. For the present, it is sufficient to indicate what strong reasons there are for assuming that

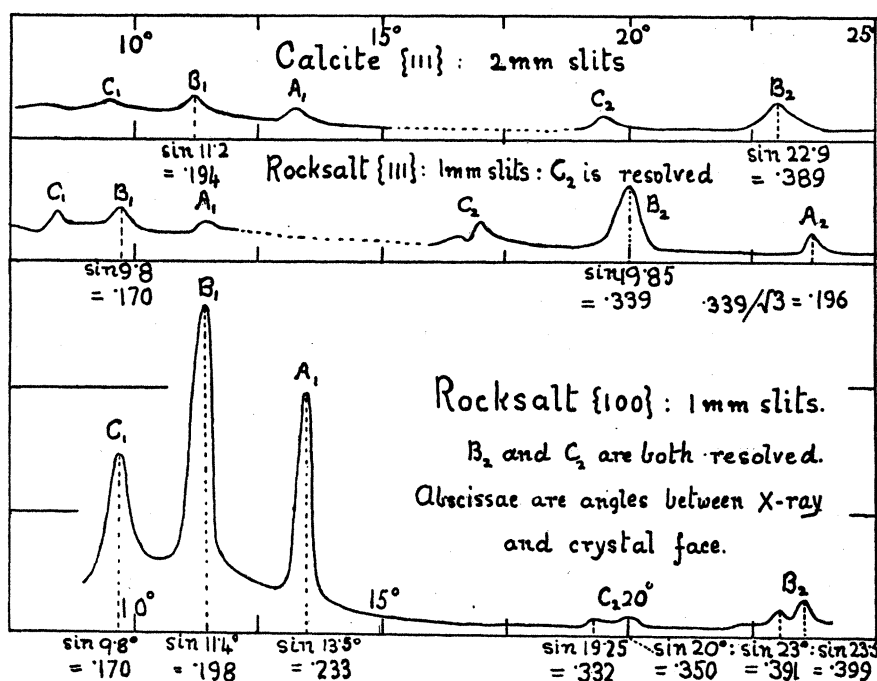


FIG. 16.

the distances d for the various faces can be accurately compared, by finding the angles at which these peaks occur.

It has been seen that the patterns given by potassium chloride, zincblende, fluor spar, and calcite can be ascribed to diffraction by points of a space lattice. It is now desired to compare the dimensions of the lattices of these crystals; since the absolute value of the wave-length λ of the radiation which forms the peaks is as yet unknown, the dimensions of each lattice will be expressed in terms of λ as unit.

Since now both the form and the dimensions (in terms of λ) of the elementary parallelepiped are known, for the space lattice arrangement of

272 Mr. W. L. Bragg. *The Structure of Some*

diffracting centres of these crystals, it is possible to calculate the volume of this parallelepiped; the volume is that associated with each point of the lattice, it is the inverse of the number of points per unit volume. A multiplication of this volume by the density of the crystal gives the mass associated with each diffracting centre, and it is to be expected that the comparison of these masses (for different crystals) will give some idea as to whether the centre consists of atoms, molecules, or groups of molecules. The results of these calculations for the various crystals are set forth in the table below:—

In this table—

θ = glancing angle of B peak, 1st order.

d = distance between planes parallel to the face investigated.

V = volume of elementary parallelepiped, calculated from this value of d and a knowledge of the nature of the lattice.

ρ = density of crystal.

M = molecular weight of substance.

Table X.

Crystal.	Lattice.	Face.	θ .	$\frac{d}{\lambda}$.	$\frac{V}{\lambda^3}$.	ρ .	M .	$\frac{V\rho}{\lambda^3 M}$.
Sylvine, KCl	Simple cubic.....	(100)	10·2	2·86	23·4	1·97	74·5	0·605
		(111)	18·0	1·62	22·2			
Rock-salt, NaCl...	Face-centred cubic ...	(100)	11·4	2·53	32·5	2·15	58·5	1·22
		(110)	16·0	1·82	33·9			
		(111)	9·8	2·95	33·5			
Zincblende, ZnS...	„ „ ...	(110)	16·5	1·76	30·8	4·06	97·0	1·28
Fluorspar, CaF ₂ ...	„ „ ...	(100)	11·7	2·46	29·8	3·18	78·0	1·18
		(111)	10·3	2·79	28·3			
Calcite, CaCO ₃ ...	Rhombohedral	(100)	10·5	2·74	44·8	2·71	100·0	1·22
		(111)	11·2	2·60				
Iron pyrites, FeS ₂	Face-centred cubic ?*	(100)	12·1	2·39	27·3	5·03	120·0	1·15

* The interference pattern of this crystal has not yet been obtained.

The last column gives the value of $V\rho/\lambda^3 M$, the mass associated with each diffracting centre divided by the molecular weight of the substance. This quantity is, therefore, proportional to the number of molecules associated with each centre. For each of these crystals, with the exception of potassium chloride, this quantity is the same within the errors* of experiment, showing

* It must be remembered that in calculating this quantity, any percentage error in the value for $\sin \theta$ is trebled, since $\sin \theta$ is raised to the third power.

Crystals as Indicated by their Diffraction of X-rays. 273

that in all these crystals the number of molecules associated with each diffracting centre is the same. Taking into consideration the very different constitution of these crystals, this fact seems to point to the association of one molecule, and one alone, with each diffracting centre; and since in zincblende, fluorspar, and calcite the molecule contains only one heavy atom, the conclusion is arrived at that the space lattice which the diffracting pattern indicates is that formed by the individual zinc or calcium atoms of these crystals.

Potassium chloride forms an apparent exception to this rule, for it has a value for $V\rho/\lambda^3M$ half that given by the other crystals. The reason for this is clear when it is remembered that in potassium chloride there are two atoms of very nearly equal atomic weights. Each molecule provides two diffracting centres, these being arranged on the simple cubic space lattice. The mass associated with each centre is not that of a molecule, but half of this quantity, and again it is single atoms, but now of two kinds, which form the points of the diffracting space lattice.

It is clear that the argument given here cannot pretend to be a complete proof of this important point. It is conceivable, for example, that in all these crystals it just happens that the molecules are grouped together in fours, and that these groups form the diffracting centres. It is easy to picture such an arrangement for the alkaline halides, in fact this is the arrangement given to all such binary compounds by the theory of closest packing by Pope and Barlow. Their arrangement would explain satisfactorily the patterns and peak relations of rock-salt, zincblende, and potassium bromide and iodide, for the black and white centres of the diagram given in fig. 8 are represented by tetrahedra composed of four spheres corresponding to atoms of either nature. This would also involve, however, the grouping in fours of the calcium atoms in calcite, and considerable difficulty is experienced in picturing an arrangement which does this. A similar difficulty arises in the case of fluorspar. Potassium chloride is also hard to account for on this arrangement, if it is granted that in this substance potassium and chlorine act almost identically on the X-rays, for the atoms are in the closest packed arrangement of the face-centred cube, while the diffraction pattern is characteristic of the simple cubic lattice. Many more comparisons of crystals are necessary to confirm this point, in the meantime it will be assumed that the simple structure correctly represents the truth, and that the diffracting centres are single atoms.

It has been seen how the comparison of the angles of reflection of a peak from various faces of the same crystal gives information concerning the space lattice structure of the crystal. Further information can be got by studying the dimensions of these peaks. For instance, the curves for two of the three

primary planes (100), (110), (111) of rock-salt are given in fig. 16* and a reference to these curves will show the very marked difference which there is between the curves for the face (100) and that for the face (111). The (100) curve shows very marked first-order peaks, much smaller second-order peaks, and the merest indication of the peaks of the third order. The (111) curve on the other hand shows the second-order peaks very much stronger than those of the first order.

This difference of the curves corresponds to a difference in the nature of the planes parallel to these faces of the crystal. In the arrangement of black and white points given in fig. 8, it will be seen that the successive planes parallel to (100) contain equal numbers of black and white points; the same is true for the planes (110), which also give a strong first-order reflection. The planes parallel to (111), on the other hand, contain alternately all blacks and all whites. The black points alone form a face-centred lattice, for which the (111) planes are further apart than the (100) planes in the ratio $2/\sqrt{3}$. Thus the small first-order peaks reflected from the (111) face of rock-salt correspond to a periodicity of black planes alone, parallel to (111), the planes containing the heavy chlorine atoms. The presence midway between these planes of the planes containing sodium atoms does not completely destroy this reflection of the first order, but it goes a long way towards doing so, while of course the reflection of the second order is reinforced and gives a large second-order peak. This explains the abnormal relative magnitudes of the (111) peaks of different orders as compared with those reflected from the faces (100) and (110).

In accordance with this, it is found that if the sodium is replaced by potassium, the first-order peak reflected from the (111) face becomes too small to be detected, the (111) curve for sylvine appears to have a peak of the first order, at an angle corresponding to planes $1/\sqrt{3}$ as far apart as the planes parallel to (100). In fact, the peaks are where they should be for the simple cubic space lattice.

This argument may be summed up as follows: The arrangement of the heavy atoms of these crystals (potassium chloride with its two equal atoms being an exceptional case) is that of the space lattice which is the skeleton of the crystal, one molecule containing one heavy atom being associated with each point of the lattice. The first order peaks of the reflection curves are in the positions which theory would give for this space lattice, but the relative magnitudes of the peaks of the first and second orders on any curve are influenced by the positions of the lighter atoms in the crystal structure. If

* For the experimental evidence in support of this part of my argument I am indebted to my father.

Crystals as Indicated by their Diffraction of X-rays. 275

these lighter atoms are so disposed as to lie on the planes of the heavy atom space lattice parallel to the face investigated, then the reflection curve may be said to be of the normal type, it will have large peaks of the first order and small ones of the second. If the lighter atoms are arranged on planes situated halfway between the planes of the lattice, the first-order peaks will be diminished and those of the second order reinforced.

The curves for the faces (100) and (111) of fluorspar show this effect in a very marked manner (fig. 17). This crystal has as its skeleton the face-centred cubic lattice, the points of the lattice being represented by the calcium atoms. The fluorine atoms are so disposed that the reflection from

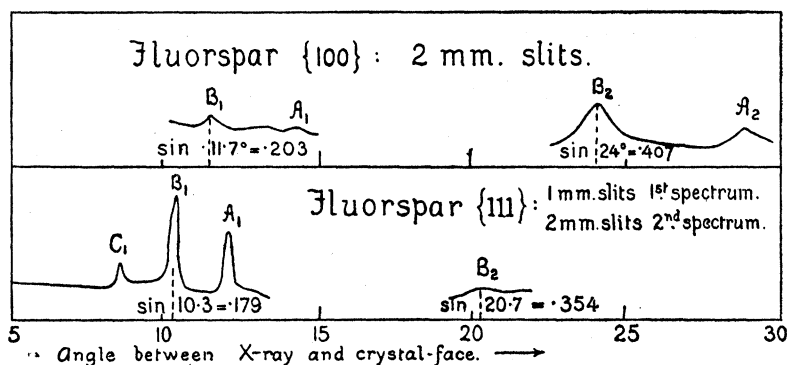


FIG. 17.

the (111) planes is now of the normal type, in strong contrast to the curves for rock-salt. On the other hand, the first-order reflection from the face (100) has almost disappeared. The fluorine atoms must be arranged so as to lie on or near the (111) planes of the fundamental lattice, not on the planes (100) as are the sodium atoms of rock-salt. The calcite curves given in fig. 16 show that for this crystal it is the (100) planes which give normal reflection, the curve for the face (111) being very like that for the face (111) of rock-salt.

It is hoped that an examination of the reflection from various faces of all these crystals may lead to the discovery of the exact positions of the lighter atoms in the crystal structure; as yet the experimental results are very incomplete. The results obtained so far seem to fix with some certainty the arrangement of the heavy atoms of these simple crystals, and in the case of the alkaline halides it is hoped that the positions assigned to atoms of both kinds are at any rate close approximations to the truth. A slight symmetrical distortion of the arrangement, which would reduce the crystal symmetry, would not affect any of the results which have been obtained here.

The analysis of crystal structures given here was initially undertaken with

276 *Crystal Structure as Indicated by Diffraction of X-rays.*

the object of discovering the absolute wave-length in centimetres of the homogeneous radiations issuing from the X-ray bulb. The positions of the peaks on the curves gave the wave-length of the corresponding radiations in terms of the dimensions of the crystal space lattice. As long as the complexity of the unit associated with each point of the lattice is unknown, the absolute wave-length cannot be calculated. If the arrangement here assigned to the alkaline halides is right, the dimensions of the lattice can be given in centimetres, for the mass associated with each centre of the lattice can be calculated from the known mass in grammes of the hydrogen atom.

For rock-salt, mass of 1 molecule of NaCl = $58.5 \times 1.64 \times 10^{-24}$; therefore

$$58.5 \times 1.64 \times 10^{-24} = V\rho = 33.3 \times 2.15 \times \lambda^3,$$

$$\lambda^3 = 1.34 \times 10^{-24}, \quad \lambda = 1.10 \times 10^{-8} \text{ cm.}$$

From the value for λ , and that for d/λ given in Table X, the dimensions of the lattice for any crystal in this table can be calculated.

Summary.

For a number of simple crystals the interference patterns can be ascribed to diffraction of a "white" radiation by a set of points on a space lattice. Each of these points is a single atom; if one atom in the molecule is at least twice as heavy as any of the others, it is the lattice formed by these atoms alone which the diffraction pattern reveals. Two atoms of nearly the same atomic weight are nearly equivalent as diffracting centres. The lighter atoms of the molecule are not grouped closely round the heavy atom forming the diffracting space lattice, but occupy intermediate positions. For instance, in sodium chloride the sodium atom has six neighbouring chlorine atoms equally close with which it might pair off to form a molecule of NaCl. The reflection curves and interference patterns given by the alkaline halides agree in assigning the same structure to these salts, the atoms being arranged on a simple cubic space lattice in such a way that rows parallel to the cubic axes contain alternate atoms of either kind. The association of a single heavy atom with each point of the space lattice is indicated by the fact that the mass of each point is proportional to the molecular weight of the substance when each molecule contains one heavy atom. This relation is got from the reflection curves of different crystals. A knowledge of the mass of a hydrogen atom makes it possible to calculate the actual dimensions of a crystal lattice, and so to find the wave-length in centimetres of the homogeneous components of the X-ray beam, this being the object for which these analyses of crystal structure were undertaken.

W. L. Bragg.

Roy. Soc. Proc., A, vol. 89, Plate 10.

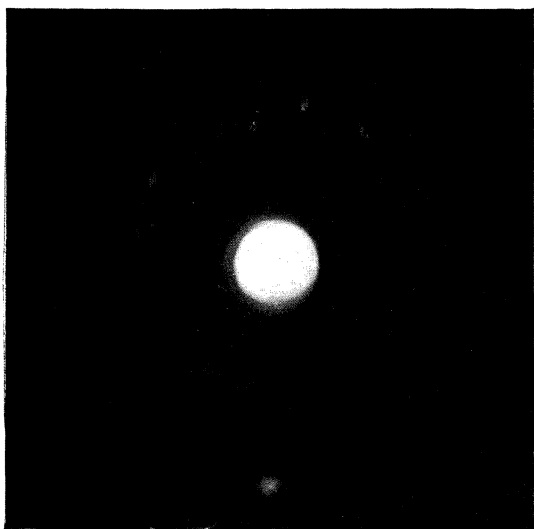


FIG. 2.—Potassium chloride.

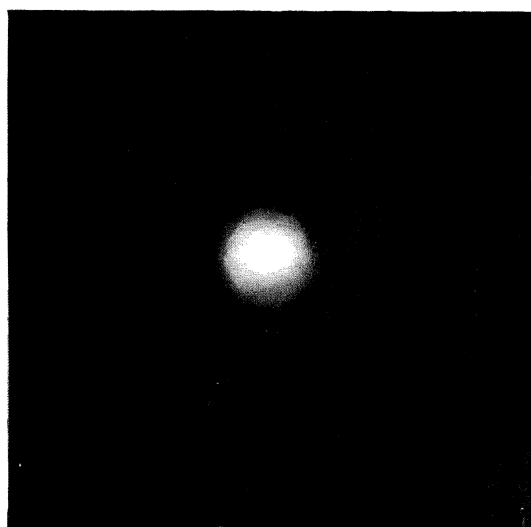


FIG. 8.—Rock-salt, 2.5 mm. thick.

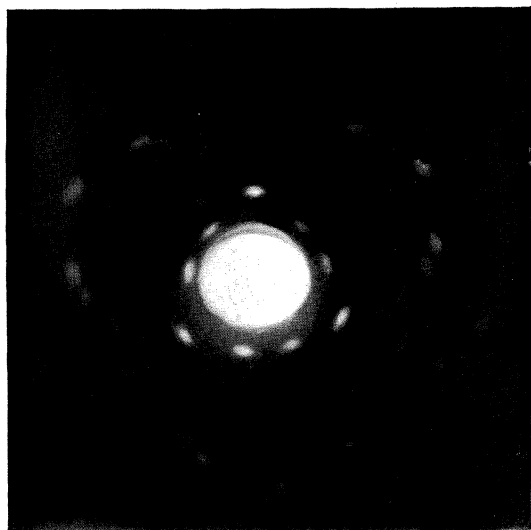


FIG. 11.—Fluorspar.



FIG. 15.—Rock-salt.

The Structure of the Diamond.

277

In conclusion I should like to express my indebtedness to Prof. Pope for his sympathetic interest and generous assistance. Dr. Hutchinson, with the greatest kindness, has overcome the only experimental difficulties connected with this subject by supplying the necessary crystal sections; but for his help it would have been impossible to obtain the very large number of photographs used in the investigation. These photographs were obtained at the Cavendish Laboratory, and I wish to thank Prof. Sir J. J. Thomson for his kind interest in the experiments. The measurements with the X-ray spectroscope were, as already stated, made by my father in the laboratory of the University of Leeds.

The Structure of the Diamond.

By W. H. BRAGG, M.A., F.R.S., Cavendish Professor of Physics in the University of Leeds, and W. L. BRAGG, B.A., Trinity College, Cambridge.

(Received July 30, 1913.)

There are two distinct methods by which the X-rays may be made to help to a determination of crystal structure. The first is based on the Laue photograph and implies the reference of each spot on the photograph to its proper reflecting plane within the crystal. It then yields information as to the positions of these planes and the relative numbers of atoms which they contain. The X-rays used are the heterogeneous rays which issue from certain bulbs, for example, from the commonly used bulb which contains a platinum anticathode.

The second method is based on the fact that homogeneous X-rays of wave-length λ are reflected from a set of parallel and similar crystal planes at an angle θ (and no other angle) when the relation $n\lambda = 2d \sin \theta$ is fulfilled. Here d is the distance between the successive planes, θ is the glancing angle which the incident and reflected rays make with the planes, and n is a whole number which in practice so far ranges from one to five. In this method the X-rays used are those homogeneous beams which issue in considerable intensity from some X-ray bulbs, and are characteristic radiations of the metal of the anticathode. Platinum, for example, emits several such beams in addition to the heterogeneous radiation already mentioned. A bulb having a rhodium anticathode, which was constructed in order to obtain a radiation having about half the wave-length of the platinum characteristic

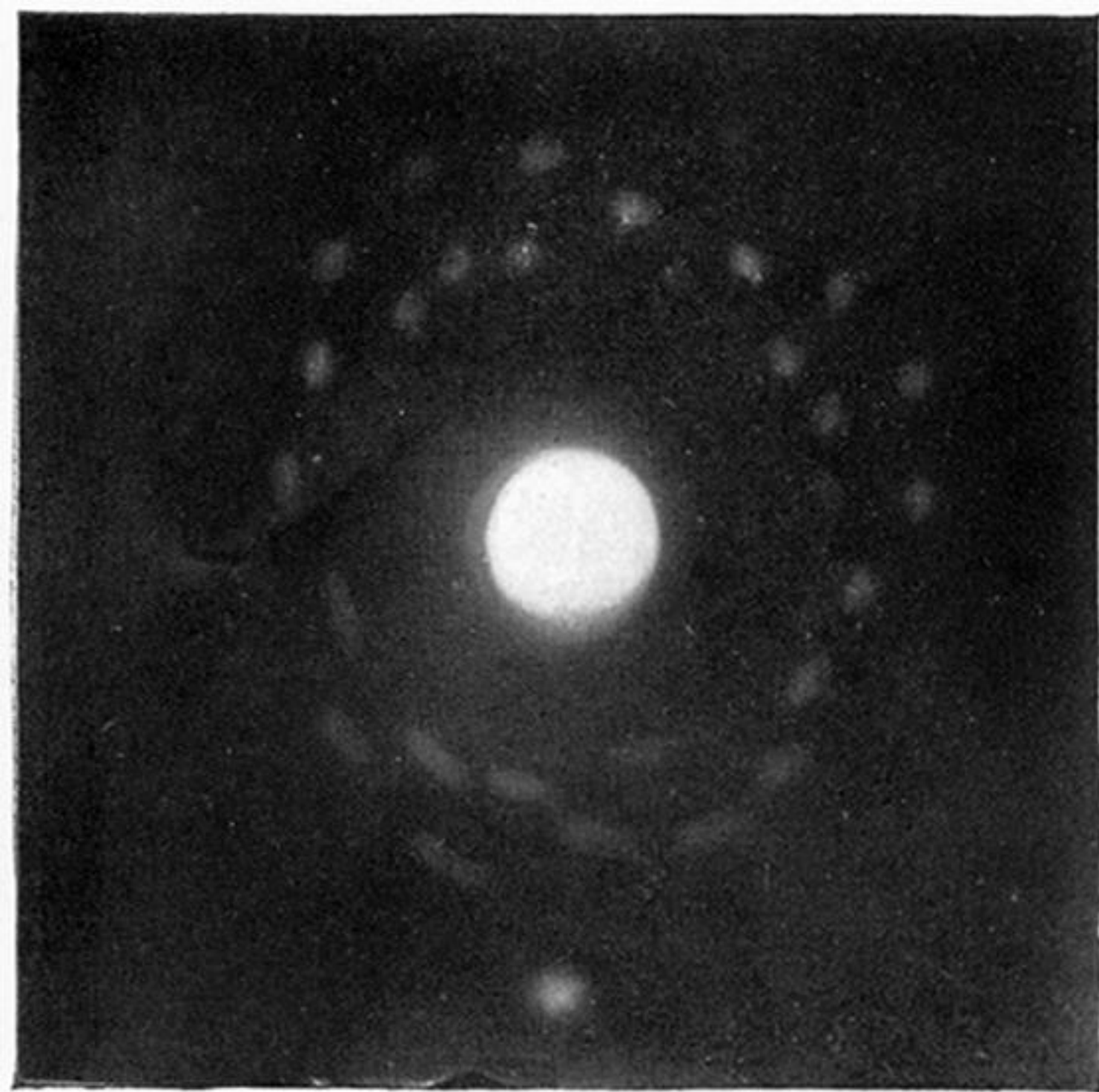


FIG. 2.—Potassium chloride.

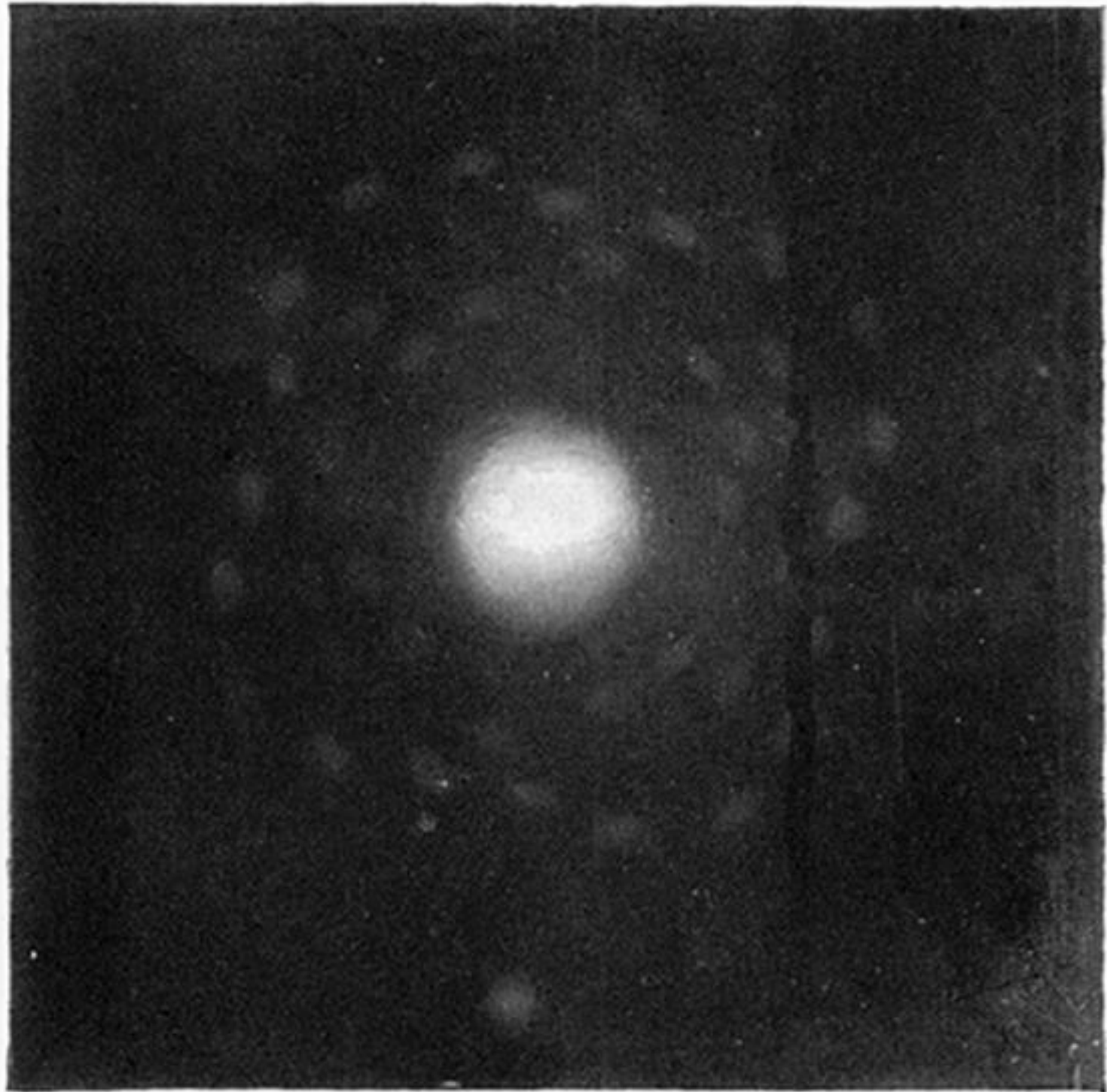


FIG. 8.—Rock-salt, 2·5 mm. thick.

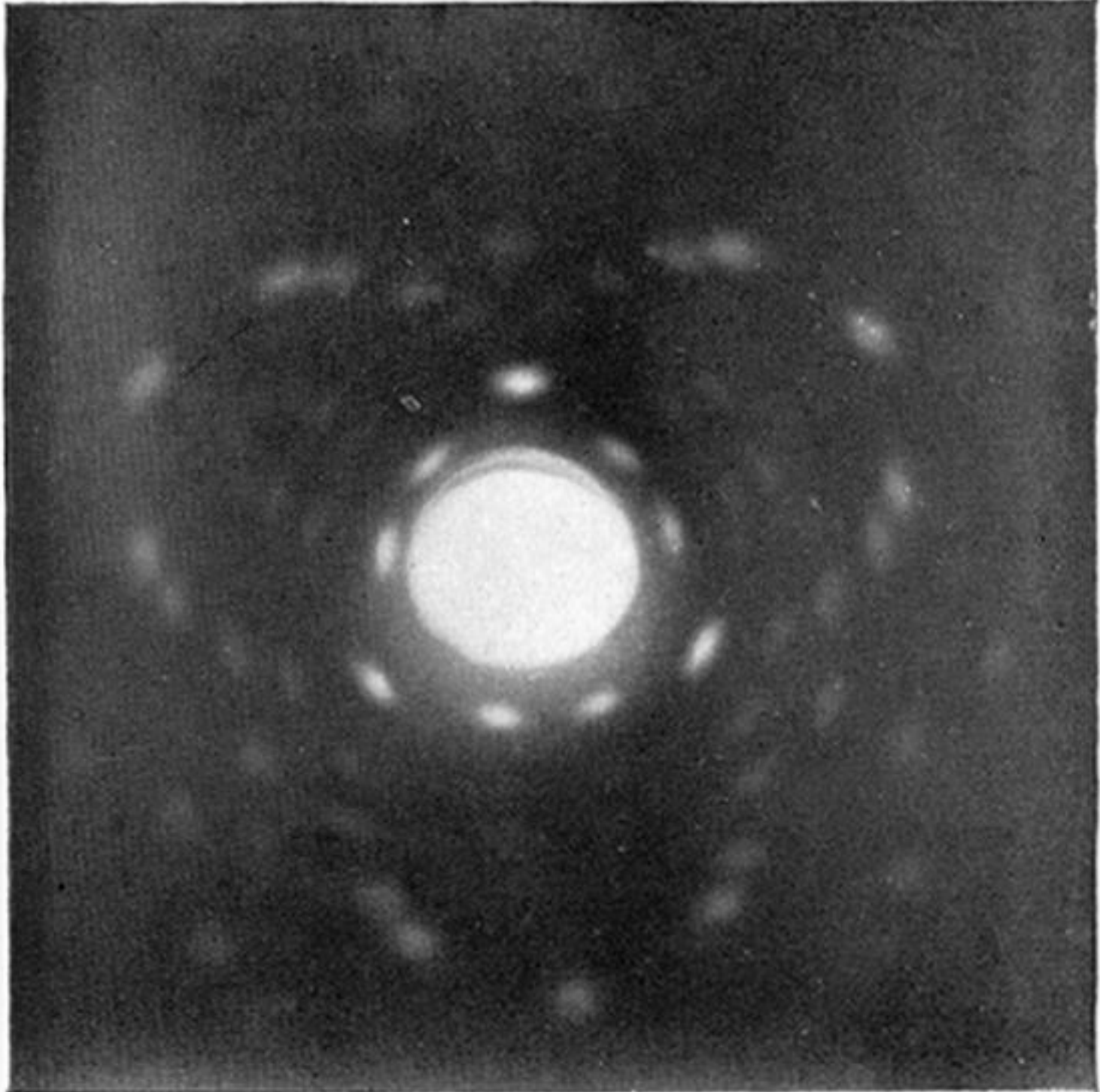


FIG. 11.—Fluorspar.

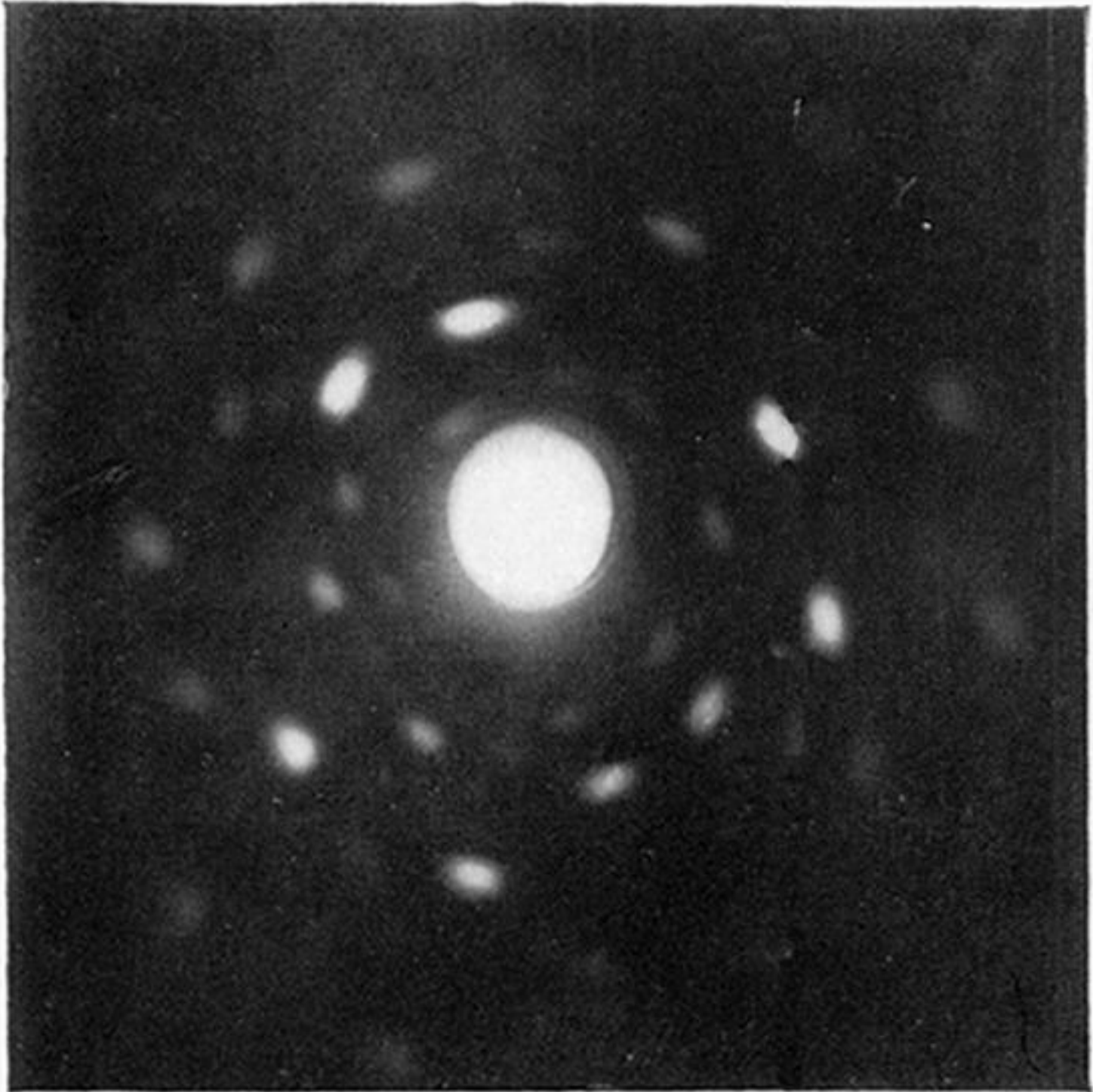


FIG. 15.—Rock-salt.