The Copy
Analytic Theory
of
Point Systems
by

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MALET STREET, LONDON, W.C.1.

1923

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"NOTHING EXISTS EXCEPT ATOMS AND EMPTY SPACE-ALL ELSE IS OPINION" - DEMOCRITOS

OCCASIONAL PAPER No.1

from the

DEPARTMENT OF CRYSTALLOGRAPHY

BIRKBECK COLLEGE (UNIVERSITY OF LONDON)

MALET STREET, LONDON WC1E 7HX

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PREFACE

In 1923, Sir William Bragg received the following letter from the mineralogist, Arthur Hutchinson in Cambridge:

Dear Sir William Bragg

25th June 1923

I am venturing to write to you on behalf of a pupil of mine, Bernal by name, whose work on point systems has, I think, been sent to you - Bernal is I think quite a remarkable person; he is a shy, diffident, retiring kind of creature, but something of a genius. He attended my course on Elementary Crystallography and I realized that he was interested and was taking things in quickly. I did not however realize (and he never let on) that he had got so keen that he spent the whole of his next vacation in developing a method of dealing with point systems in the hope that it might be useful in X-ray work! When therefore, he suddenly appeared and deposited on my table a thick type-written MS., rather with the air of a dog bringing a poached rabbit to his master's feet, I was quite amazed - of course I make no pretence of being able to appraise its merit or even its usefulness - still it seemed to me a remarkable effort for an undergraduate in his third year - and Professor H.F.Baker was much interested in it and I believe thinks well of it...

This paper was thus written by John Desmond Bernal (1901-1971) when he was 21. It was submitted as a prize essay to Emmanuel College, Cambridge where Bernal was an undergraduate and earned him the Sudbury Hardyman prize of £30, but it also got him a post with Sir William Bragg and set him on a career in crystallography. The paper was then presented to the Cambridge Philosophical Society on 7th July 1923 as "The Analytic Theory of Crystals" but, although it was accepted, the paper was, on account of its length, never published. One manuscript copy, typed, we believe, by Mrs Eileen Bernal, has circulated in this department for many years, surviving precariously, but we now hasten to publish it in facsimile to avoid further danger of its loss.

Some of the circumstances of the production of this paper are described at length by Professor Dorothy Hodgkin, O.M., F.R.S., who was the earliest of Bernal's students and co-workers during his period in the crystallographic laboratory at Cambridge, in her biographical notice of Bernal (Biographical Memoirs of Fellows of the Royal Society, 26, (1980) which we quote for Prof. Hutchinson's letter and to which reference should be made for details of Bernal's scientific career.

The accompanying article, "X-rays and Crystal Structure" was written by Bernal in 1929 for the 14th Edition of the Encyclopaedia Britannica (and is here reproduced by kind permission of the copyright holders). It clearly follows from Bernal's essay. Bernal also wrote the corresponding article for the 1953 edition of the Encyclopaedia (Vol. 6, pp. 809-829. It ends with the sentences: "The beating out of metal under the hammer, the brittleness of glass and the cleavage of mica, the plasticity of clay, the lightness of ice, the greasiness of oil, the elasticity of rubber, the contraction of muscle, the waving of hair and the hardening of a boiled egg are among the hundreds of phenomena that had already been completely or partially explained. They were an earnest of the millions of others, old or new, that still had to be explained." In the period Bernal prepared a further version for the succeeding edition but, regrettably, this was not published because it was too long and had too many illustrations. Evidently the successes of crystallography in explaining the material world and Bernal's enthusiam had outrun commercial prudence!

J.D.Bernal was elected a Fellow of the Royal Society in 1938 for his work on the elucidation of the structures of biological molecules by the methods of X-ray crystallography and in the same year he succeeded P.M.S.Blackett as Professor of Physics here at Birkbeck College in the University of London. Almost immediately Bernal was drawn into the war but in 1946 the Birkbeck College Research Laboratory for bio-molecular structure was founded in two old houses at 21/22 Torrington Square (now the site of the library of the School of Oriental and African Studies). This was formally opened by Sir Lawrence Bragg on 1 July 1948 for which occasion Bernal wrote: "the central theme of the laboratory is the application of physical methods to the understanding of the structures and reactions of molecules in biological systems". The formal teaching of crystallography (M.Sc. by examination) began at Birkbeck also in 1948 and has continued ever since. In 1964 the Laboratory became the Department of Crystallography (moving into the new extension building and separating from the Department of physics) with Bernal as its first Head and first Professor of Crystallography, bur in the same year Bernal suffered the first of a series of strokes. On his retirement in 1968 he was succeeded by C.H.Carlisle and in

1978 by T.L.Blundell, the present occupant of the established chair of crystallography and Head of the Department.

We have invited Professor Rolph Schwarzenberger of Warwick University to give an assessment of this, Bernal's first paper, which, by accident, has remained hitherto unpublished, and we are most grateful for his note which puts the paper into perspective and explains quaternions.

We believe that nothing could be more appropriate as Occasional Paper No.1 from the Department of Crystallograhy which Bernal founded to continue the studies which he himself had advanced so much.

Alan Mackay

July 1981

INTRODUCTORY NOTE

R.L.E. Schwarzenberger Science Education Department University of Warwick

One way to assess the novelty of Bernal's manuscript is to place it side by side with the two books which he himself used:

H.HILTON. Mathematical Crystallography and the theory of groups of movement, Clarendon Press, Oxford 1903.

P.NIGGLI. <u>Geometrische Kristollographie des Diskontinuums</u>, Borntraeger, Leipzig 1919.

The two books have in common that they include the listing of the 230 space groups as it was published by Schönflies* in 1891 (Niggli copies Schönflies exactly whereas Hilton changes some nomenclature in translation and alters the order in which the crystal systems occur. Bernal follows Hilton). They differ in that Hilton attempts to give a full proof that there are precisely 230 possibilities whereas Niggli gives proofs of general results, listings of groups and much additional information about each group (along the lines of the future International Tables). Hilton is more interested in group theory than in crystallography and uses geometrical methods which stem directly from those of Schönflies, whereas Niggli uses algebra more and deals also with crystal form and with deformations of structure.

It is worth recalling that neither Schönflies nor Fedorov nor Barlow succeeded in getting the number of distinct groups correct at their first attempt: the list of 230 space groups was achieved only as a result of mutual checking between Schönflies and Fedorov. I do not believe that Hilton would have done better, had he not been writing with the list of Schönflies in front of him, because his method is not guaranteed to catch every possible special case of existence or equivalence. Thus Bernal was inspired by Niggli's more analytic approach to try to make more precise the "simple and geometric" qualitative proof contained in Hilton's book. In this approach Bernal was following very closely in the footsteps of Fedorov who had written over 30 years earlier:

^{*}Kristallsysteme und Krystallstruktur, B.G.Teubner, Leipzig, 1891.
The second revised edition appeared as Theorie der Kristallstruktur-ein Lehrbuch, Borntraeger, Berlin, 1923. There is no evidence in the manuscript of Bernal having consulted Schonflies directly - in any case Hilton is considerably clearer.

"...here, for the first time, the symmetry of figures is expressed in analytical terms and in this way the theory of symmetry is itself introduced into the realm of analytic geometry. Originally I intended to find analytic terms for the symmetry of finite regular systems. I was prompted to do this by the difficulty of interpreting Sohncke's derivations.....an error which remained unnoticed for a long time by the author himself.....this could hardly have happened if these systems had been expressed in analytical terms"

(E.S. Fedorov "Symmetry of Finite Figures" 1889 translated by D. Harker 1971)

Similarly Bernal realised that more precise and analytic methods were required for the qual itative listing (Sohncke, Schönflies, Barlow, Hilton) to become useful in the new crystallographic applications. In the remainder of this note I would like to draw attention to three ways in which Bernal notably achieved this aim.

The first important improvement made to Hilton's proof is the decision to work in vector space (i.e. with fixed origin) rather than in affine space. Hilton follows Schönflies in writing, for example, $A(\alpha)$ to denote a rotation through angle α about an $3 \times 10^{\circ}$ A, or S(t) to denote a glide transformation with translation component t lying in the plane of reflection S. But the axis A and the plane S need not pass through the origin, which is good for nice qualitative pictures of crystals but bad for precise analytic proofs of the mathematics. Bernal chooses an origin and assigns each affine transformation

$$X \longrightarrow eX + c$$

its linear part **Q** and its translation component **c**. The importance of this change for the development of mathematical crystallography is in no way diminished by the fact that, under the steadily increasing influence of modern algebra, many other mathematicians did the same thing quite naturally and most crystallographers do so today.

This leads to the most striking aspects of the manuscript: the influence of modern algebra in the discussion of quadratic forms (in Chapters II and III the symbol SXY is the scalarproduct of X and Y) and in the use of quaternions throughout. In crystallography the linear part of a symmetry is, of course, a 3x3 matrix determined by coefficients. The fact that Q preserves lengths and angles imposes 6 conditions so only 3 degrees of freedom are left for Q. Clearly a more precise analytic approach would benefit from a more economic method of presentation of 3 parameters. It was fairly well known among theoretical physicists and mathematicians that all such linear parts arise from transformations of the form

$$X \longmapsto \pm q X q^{-1}$$

where q is a unit quaternion (the correspondence between

unit quaternions and linear parts is actually not one-one, because -q determines the same transformation as q; this does not cause any confusion in practice). Most readers of this note will be familiar with this fact but, for those who are not, a brief note on quaternions is appended which covers those facts assumed without comment by Bernal in Chapters II and III. Note that the quaternion notation - unlike matrix notation - allows angles of rotation, axis of rotation, plane of rotation to be read off immediately. This is a great advantage when trying to decide whether two groups are or are not equivalent.

The third important improvement is the explicit mention of specialisation: no doubt influenced by the algebraic geometry of the time. This is merely the very simple observation that, for example, a tetragonal lattice is a special case of a orthorhombic lattice. This observation is present but less explicit in Hilton, and explains why Hilton (and so also Bernal) deals with the tetragonal system immediately after the orthorhombic system (Schönflies has the mombohedral system in between, presumably on the ground that 12 is between 8 and 16).

The effect of these three improvements is that far more facts can be established as general theorems applicable to many crystal systems. Here Bernal is following the example set by Niggli in contrast to Hilton's insistence on a separate discussion for each crystal system. It follows too that the listing of space groups becomes essentially a listing of the relevent translation components which can be handled algebraically. In modern language, Bernal is listing the relevant cocycles to determine a first cohomology group.

In summary, Bernal has rewritten the proof (Sohncke, Schönflies) which he found in Hilton but has brought to it the more analytic attitudes of a quite different crystallographic tradition (Möbius, Fedorov, Niggli). His excellent knowledge of current mathematics yields an improvement upon the treatment of Hilton, 20 years earlier, and comes close to foreshadowing the cohomological work of Zassenhaus, 20 years later.

Kolph Schwarzenberger April 1981 NOTE ON QUATERNIONS

Any set of 4 real numbers a, b, c, d can be displayed conveniently as a single quaternion a+bi+cj+dk. The chief advantage of the notation is the ability to multiply using the idenitities $i^2=j^2=k^2=-1$ and ij=-ji=k. Many properties are analogous to those of complex numbers; for example if q=a+bi+cj+dk then the conjugate $\bar{q}=a-bi-cj-dk$ satisfies $\bar{q}q=a^2+b^2+c^2+d^2$.

If x is a pure quaternion then the transformation $e : x \longmapsto qxq^{-1}$

sends \bar{X} to another pure quaternion because $\bar{q}xq^{-1} = \bar{q}^{-1}\bar{x}\bar{q} = q\bar{x}q^{-1} = -qxq^{-1}$

Moreover it is easily shown to preserve lengths and angles. The vector X is fixed under the transformation if and only if qX=Xq. Inspection shows that this happens if and only if X is a multiple of b'i+c'j+d'k. Thus q is a rotation about the axis (b', c', d'), and it can be checked that the angle of rotation is 2q.

Similarly the transformation

$$-e: x \longrightarrow -qxq^{-1}$$

is a combination of a reflection and a rotation, that is a symmetry of the second kind.

The power of this notation can be seen when considering composition. If the rotation $X \longmapsto q_1 X q_1^{-1}$ is preceded by the rotation $X \longmapsto q_2 X q_2^{-1}$ then the composite rotation may be represented by the transformation

$$x \mapsto q_x xq_x^{-1} \mapsto q_1 (q_x xq_x^{-1})q_1^{-1}$$

or precisely the transformation $X \longleftrightarrow q_3Xq_3^{-1}$ where $q_3 = q_1q_2$. This is a very much simpler formula for the composition of two rotations than that of Euler and Rodrigues quoted by Hilton.

Preface

I was led to the subject of the present paper by a consideration of the X-ray analysis of crystals. The general uncoordinated and tentative aspect of the methods used seemed to point to an unsuitable geometric groundwork. When Schoenflies, Von Fedorof and Barlow solved the final problem of the 230 types of homogeneous structures there conclusions were purely geometric and there seemed no immediate prospect of applying them to actual crystal structure. As it was only necessary to distinguish one such structure from another, a qualitative basis was sufficient. But this qualitative basis did not meet the needs of X-ray analysis of crystal structure, and the pioneers in this field consequently fell back upon simple and geometric methods which they evolved in the course of their work.

What was wanted, it seemed to me, was an analytic theory in which the structure of a crystal could be represented by a quantitative formula, and the analysis of this structure could be reduced to the solution of cortain equations. It occurred to me that the application of simple vector and quaternion calculus would supply the need of experimentalists while at the same time providing yet another solution to the problem of homogeneous structures.

This solution occupies the first six chapters of the paper. It is given in extremely condensed form, and the absence of examples and diagrams may make it difficult to follow the geometric meaning of the various expressions. In this connection references under the heads of Classes and Systems should be made to Hilton's <u>Mathematical Crystallography</u>. Chapters VII and VIII are deductions from the theory which lead to Chapter IX on the X-ray analysis.

Circumstances prevented this Chapter from being as full as was originally intended, especially with respect to the lack of examples and the scant attention paid to the Laue and Hull methods, deficiencies which I intend to make good at a later date.

As the theoretical part has been written independently the absence of references will be understood: the only works to which I am indebted are Hilton (ibid) and Niggli, Analytische Geometrie der Discontinuums, from which I have takensome of the proofs in Chapter III. In Chapter IX I have relied almost entirely on Bragg's X-rays and Crystal Structure, and in view of the forthcoming appearance of the 2nd edition of this work, the elementary nature of the Chapter is perhaps not unfortunate.

POINT SYSTEMS

1.1 Point Systems

Consider a system of points in an n dimensional continuum.

The position of any point is determined by the vector I representing the line drawn from an arbitrary origin 0 (not necessarily a point of the system) to the point. This point is called the point I.

The whole system is determined when the origin 0 and the vectors corresponding to all the points are given. Thus the system is completely determined by

 X_1, X_2, X_3 , X_r written for short $/X_r$ /X, is called the aspect of the system from 0.

.2 If n independent vectors are chosen. i.e. if A_1, A_2, \dots, A_n . can be chosen such that

 $x_1A+x_1A_1+x_2A_2+\dots$ $x_nA_n\neq 0$ unless $x_1=x_1=\dots=x_n=0$ then x_1 can always be written

 $x_{ii}A_i + x_{ii}A_i + x_{ii}A_i + \dots + x_{ni}A_i \quad .$ and the aspect of the system represented by

$$/\mathbf{z}_{1}^{A_1} + \mathbf{x}_{2}^{A_2} + \dots + \mathbf{x}_{n}^{A_n}$$

The vectors A_1, A_2, \ldots, A_n , are called the coordinate system or reference vectors.

The scalar coefficients $\mathbf{x}_{i_1}, \mathbf{x}_{j_1}, \dots, \mathbf{x}_{p_j}$, are called the coordinates of the point \mathbf{x}_i and are often used to denote the point \mathbf{x}_i .

Discontinuous Systems.

If for two points of the system x, x,x, x, x,x, all the positive scalar differences

are either =0 or e, when e ish finite positive scalar, the system is said to be discontinuous. In everything that follows all systems are assumed to be discontinuous.

Homogeneous Systems.

If there exists at least n points whose vectors are independent and from which the aspect of the system is the same, i.e. for which $/I_r$ represents the aspect of the system; then the system is called homogeneous.

Let the points

$$\begin{array}{lll} B_i = & b_n A_1 + b_n A_2 + \dots & b_n A_n \\ B_k = & b_{ik} A_i + b_{ik} A_k + \dots & b_n A_n \end{array}$$

 $B_n = b_{i,k}A_i + b_{i,n}A_i + \cdots + b_{n,k}A_n$, be such a set of points then since the system has the same aspect from $B_i \cdot B_i \cdot B_{i,i}$ as it has from 0 there is corresponding to any point $x_i, x_i, \dots x_n$.

the points
$$x_1 + b_{11}, x_2 + b_{12}, \dots, x_n + b_{n1}$$
.

$$\mathbf{x}_{i} + \mathbf{b}_{in}$$
, $\mathbf{x}_{1} + \mathbf{b}_{in}$, ..., $\mathbf{x}_{n} + \mathbf{b}_{in}$

Corresponding to these again are the points x_1+2b_1 , x_2+2b_2 , ..., x_n+2b_n , etc.

$$\boldsymbol{x}_{_{1}}+\boldsymbol{n}_{_{1}}\boldsymbol{b}_{_{1}}+\boldsymbol{n}_{_{1}}\boldsymbol{b}_{_{11}}+\ldots+\boldsymbol{n}_{_{1N}}\boldsymbol{b}_{_{11}},\quad\boldsymbol{x}_{_{2}}+\boldsymbol{n}_{_{2}}\boldsymbol{b}_{_{1}}+\boldsymbol{n}_{_{1}}\boldsymbol{b}_{_{2}}+\ldots+\boldsymbol{n}_{_{1N}}\boldsymbol{b}_{_{1N}},\quad\ldots,\boldsymbol{x}_{_{N}}+\boldsymbol{n}_{_{N}}\boldsymbol{b}_{_{N}}+\boldsymbol{n}_{_{N}}\boldsymbol{b}_{_{NN}}$$

where it /n, can have integral values positive or negative

.41

.5

Further, the coordinates of any point $x_1, x_2, x_3, \dots, x_n$, become if the point $n_n b_n + n_{i_1} b_{i_1} + \dots + n_{i_n} b_{i_n}, n_{i_1} b_{i_1} + \dots + n_{i_n} b_{i_n} + \dots$

 $\mathbf{x}_1 - \mathbf{n}_{11} \mathbf{b}_{11} - \mathbf{n}_{12} \mathbf{b}_{12} - \cdots - \mathbf{n}_{1n} \mathbf{b}_{1n}, \ \mathbf{x}_1 - \mathbf{n}_{21} \mathbf{b}_{22} - \cdots - \mathbf{n}_{1n} \mathbf{b}_{2n}, \dots$ and since there is a point with the same coordinates referred to the old origin, the system must have the same aspect from all the points

These systems have the property of having the same aspect from every point of the system. Such systems are called lattices. All lattices can be written in the form

 $/n_{i}A_{i}+n_{i}A_{i}+\cdots+n_{i}A_{n}$

when $/n_{jr}$ are integers and A_{j} , A_{j} , ..., A_{k} , a set of properly chosen vectors.

Returning to the original system; now suppose there is another point $b_{inq}, b_{inq}, \dots, b_{neq}$ isognomic with the origin i.e. such that the system has the same aspect when viewed from these two points; then the point $\mathbf{x}_i + \mathbf{n}_{in}b_{inq} + \mathbf{n}_{i1}b_{i1} + \dots + \mathbf{n}_{in}b_{in}, \mathbf{x}_i + \mathbf{n}_{in}b_{i1} + \dots + \mathbf{n}_{in}b_{in} + \mathbf{n}_{i1}b_{i2} + \dots + \mathbf{n}_{in}b_{in}, \mathbf{x}_i + \mathbf{n}_{in}b_{i1} + \mathbf{n}_{i1}b_{i2} + \dots + \mathbf{n}_{in}b_{in}, \mathbf{x}_i + \mathbf{n}_{i1}b_{i1} + \mathbf{n}_{i1}b_{i2} + \dots + \mathbf{n}_{in}b_{in}, \dots$ are points of the system. Subtracting, we have the difference of coordinates $\mathbf{n}_{inq}b_{ini} - \mathbf{n}_{i1}b_{i1}$, $\mathbf{n}_{inq}b_{ini} - \mathbf{n}_{i1}b_{i1}$,

Now none of these must be infinitensimal and this can only happen for all integral values of \mathbf{n}_{ij} if $\frac{\mathbf{b}_{inq}}{b_{i1}}$ is commensurate, extending we have $\sqrt{\frac{b_{ij}n_{ij}}{b_{ij}}}$ commensurate.

Therefore all points isognomic with 0 may be written in the form

 $p_n b_n + p_{n}b_n + \cdots + p_n b_{n}$ where $/p_{r,c}$ are rational fractions

.6 All the isognomic points of the system may be written $/p_{17}B_{1}+p_{17}B_{2}+\dots\dots+p_{n7}B_{n}.$

 p_r can always be written $1 + \frac{m_r}{n_r}$ where $1, m_r, n_r$ are all integers and $n \ge m \ge 0$ Now since $p_r \ge 0$. By are isognomic points.

The points $\frac{m_1}{n_1}, \frac{m_2}{n_1}, \cdots, \frac{m_r}{n_n}$ must belong to the system and there must be a finite number k of such points. Of these n as reference vectors independent points may be chosen. (If k(n some of the points Isognomic

B, B, canbe taken as well) The number of/points with pure fractional coefficients referred to these vectors must be less than before, and continuing the process we must arrive after a finite number of operations to a set of reference vectors in which there is only one point with fractional coefficients and this is the point

.61 All the isognomic points referred to a primitive set of vectors A_1, A_2, \ldots, A_n , can be expressed in the form

 $/1_{i_1}A_i+1_{i_2}A_i+\cdots+1_{i_n}A_n$

2000.....O. Such a Spatemais called a primitive.

where $/1_r$, take all integral values positive or negative. This lattice which includes all the isognomic points of the system with respect to the origin O is called the skelwtal lattice of the system.

primitive

The choice of an elementary set is not unique. There are except for the case (n=0) an infinite number of such sets.

If
$$A'_1 = 1_{11}A_1 + 1_{21}A_2 + \dots + 1_{q_1}A_q$$

 $A'_2 = 1_{11}A_1 + 1_{22}A_2 + \dots + 1_{q_2}A_q$

 $A'_{n}=1_{1n}A_{1}+1_{2n}A_{2}+\dots 1_{2n}A_{n}$ is such another set it must be possible to express A_{1} in the form

 $A_i=l_{i_1}'A_i'+l_{i_1}'A_i'+\dots\dots l_{i_l}'A_n' \quad \text{etc.} \quad \text{Where }/l_{rs}' \text{ are integers}$ Now the condition for this is

$$\begin{cases} 1_{i1} 1_{j_1} 1_{j_2} & 1_{j_1} = \pm 1 \\ 1_{i_1} 1_{i_1} 1_{i_2} & 1_{j_1} \\ 1_{i_2} 1_{i_3} 1_{i_5} & 1_{j_2} \\ \vdots & \vdots & \ddots & \vdots \\ 1_{j_n} 1_{i_n} 1_{i_n} & \ddots & \vdots \end{cases}$$

so that this relation must hold good for the coordinates of any primitive set expressed in terms of any other,

By an extension of this proof it can be seen that if the determinant $(I_1, \dots, I_m) \ge \pm \hbar$ the set of reference vectors A_1, A_2, \dots, A_n . is of the m th order, that is the number of proper fractional points is m and the highest value of any denominator must also be m.

.8 Component Set.

. 7

The general expression for a homogeneous system may now be written $/ (\mathbf{x}_n + \mathbf{l}_n) \mathbf{A}_1 + (\mathbf{x}_n + \mathbf{l}_n) \mathbf{A}_2 + \dots + (\mathbf{x}_n + \mathbf{l}_n) \mathbf{A}_n +$

$$/(\bar{x}_{i_{1}}^{*+1}, \bar{x}_{i_{1}}, \bar{x}_{i_{1}}^{*+1}, \bar{x}_{i_{1}}^{*+1}, \bar{x}_{i_{2}}^{*+1}, \bar{x}_{i_$$

where $/A_r$ is a primitive set. This expression represents every point of the system once and once only if $/(x_{r,j}-x_{r,j})$ are not all integers for all values of r(s constant) and of s. We each point $x_{r,i}x_{r,j}-x_{r,j}$ is seen to to be accompanied by a lattice of equivalent points; and the number of such lattices m is called the

Since there are m of such lattices the mystem is called an m lattice or m point system. The set of points $x_{12}A_1 + x_{13}A_2 + \dots + x_{16}A_n + \dots$ is called a component set of the system. One component set corresponds to each point of the skeletal lattice. Instead of $/x_{13} x_{23} x_{33} x_{33} = x_{33} /(x_{13}+1_{17}), (x_{13}+1_{13}), \dots, (x_{n5}+1_{n3})$ might have been chosen as one of the component set, it is consequently possible and sometimes useful to limit the values of the coordinates of the points in a component set. The limits most often employed are (A) $0 \le X \le 1$ and $(B) - \frac{1}{2} \le x \le \frac{1}{8}$ (A) avoids negative coordinates, (B) is more symmetrical.

CHAPTER II.

SYMMETRY

Characteristics of a Vector set

For every set of n independent vectors there exists $\frac{n(n+1)}{2}$ symmetrical of the type quadratic forms of the type Q(X) Q(XY) these forms are called the characteristics of the set.

2 Congruence

2.1

Q
$$(x_1A_1+x_2A_2+...+x_nA_n)=0(x_1A_1'+x_2'A_2'+....+x_nA_n')$$

and $Q(x_1A_1+x_2A_2+...+x_nA_n)(x_1'A_1+x_2'A_2+....+x_n'A_n)$

$$\P \ Q(\underline{x_1}\underline{A_1'} + \underline{x_2}\underline{A_2'} + \ldots + \underline{x_n}\underline{A_n'})(\underline{x_1'}\underline{A_1'} + \underline{x_1'}\underline{A_2'} + \ldots + \underline{x_n'}\underline{A_n'})$$

for all values of $/x_r$. From this it follows that if in two systems with congruent reference vectors, there corresponds to every point x_1x_2, \ldots, x_n in one there—a point x_1x_2, \ldots, x_n in the other, then the two systems are congruent and conversely.

Symmetry

If a system is such that two or more aspects of it are congruent though not in general identical, it is said to be symmetrical.

If 0, C, C' are the points from which the system has the congruent aspects then for any two points X and Y there are corresponding points $C + X', C + Y'; C' + X', C' + Y''; \ldots$ where $X, Y; X', Y'; \ldots$ are connected by the equations $Q(X) = Q(X') \ldots$

$$Q(XY) = Q(XY) \dots$$

Now X must obviously be some vector function of X consistent then with the above conditions. Writing X'=f(X) we have if Y is the point corresponding to X, 1.* if Y=X'+C we may write as the general form of the my condition of symmetry the identity.

Y = f(X)+C.

4 Symmetry in three dimensions.

Leaving at this point the study of point systems in n dimensions we may examine the form which the symmetry function f(X) takes up where n=3 that is in the ordinary space of three dimensions. In this case we may write $Q(X)=X^{\frac{1}{2}}$ and $Q(XY)\not=S.XY$ and the conditions which f(X) must satisfy become

 $f(X)^{L} = X^{L}$ and Sf(X)f(Y) = SXY

One form of f(X) which satisfies both these conditions is the quaternion transformation

 $\underline{f(X) = qXq^{-\prime}} \quad \text{where q is a quaternion}$ another is the negative quaternion transformation

 $\mathbf{f}(\mathbf{X}) = -\mathbf{q} \mathbf{X} \mathbf{q}^{-1}.$

There are no other forms which can satisfy the conditions; for since $f(X)^{*} = X^{*}$, q can always be found such that $f(X) = qXq^{*}$ and similarly q'can always be found such that $f(X) = qXq^{*}$.

then S f(X)f(X) =SqXqqXq = S XX if and only if q =q

Thus the general condition of symmetry must always take one or other of the forms $\underline{Y} = \underline{q} \underline{X} \underline{q'} + \underline{0}$ $\underline{Y} = \underline{-q} \underline{X} \underline{q} + \underline{C}$. These identities are known as symmetry relations of the first and second sort respectively

The symmetry relation Y) Sique of may always be written in the in inverse form I Sique where C sqCq Multiplying both of these expressions by q adding them and dividing the sum by two we arrive at the symmetry relation in its most symmetrical shape.

$$(Y-\frac{C}{2})q \stackrel{\bullet}{=} q(X+\frac{C}{2}) = 0$$

or $\{Y = \frac{C}{2}\}^2 q + q(X = \frac{C}{2}) = 0$ for relations of the first and second sort respectively, or more simply still

$$(Y-C)q-q(X+D) \neq 0$$

In the important particular case in which C= 0 the relation takes the simplest form of all

Yq 7 qX 3 0 .

The unsymmetrical forms are in general more easy to deal with because they involve only one constant vector, and they will be used in all the subsequent work. The other forms were only introduced to show the essential symmetry of the relations.

Combinations and Transformations of Symmetry Belations.

If a system posesses two symmetry relations

- (1) $Y = (-1)^{q} X q^{-1} + C$
- (2) $Y= (-1)^{n}QXQ^{n+1}C'$ where v is an integer odd or even and in (1) we put X=Y', we have
- •71 (12) $Y = (-1)^{q} \{(-1)^{q} X q^{-1} + C\} q^{-1} + C'$ which reduces to
 - (12) Y= (-1) Y+Y q'q Xq-'q'+(-1) q'cq'+c'

and since q'q is a quaternion whose reciprocal is q''q'' this is equivalent to another symmetry relation.

This new relation is called the somblines relation (12) . The combined relation (21)

(21) $Y = (-1)^{2} q' X q'' q'' + (-1)^{2} Q Q'' + Q''$

is in general not the same .

It should be noticed that if (1) and (2) be both relations of the first or both of the second sort their combination is an relation of the first sort; whereas if one is of the first and the other of the second sort their combination is of the second sort.

73 The combination of one relation with it self n times will always be all relation of the system so that the relation

YE (-1)qXq +C always implies the Mfurther relations
YE (-1) q Xq +nC

where n may have all integrak values positive or negative.

.78 The combination (-121)

(-121) Y= (-1)qqq Xqq'q'-(-1)qqq'Cqq'q'+qCq'+C is called the transformation of (2) by (1)

8 Reduced Symmetry Relations

In any point system we can always write

 $X=X_{lmn}+X'$; $Y=Y_{lmn}+Y'$ where $X_{lmn}=lA+mB+nC$, A,B,C being primitive reference vectors, and R_{lmn} , n integers; while X:=pA+qB+qC where p,q,r are proper fractions though not necessarily rational: similarly for Y_{lmn} and Y. The general symmetry relation now takes the form

 $Y_{l'n',p}Y=(-1)^{n'}q(X_{lm,p}X^{l'})q^{l'}+D$ (writing D for C to avoid confusion) $1^{l'}_{l,m',n'}$ are the integers corresponding to 1,m,n.

For the skeletal lattice that includes the origin X=Y=0

The relation can therefore be considered as the sum of the two rel-

relations

 $Y_{tun}=(-1)^{n}_{q}X_{tnu}^{-1}+D,$ $Y'=(-1)^{n}_{q}X'+D,$ where $\Phi+D=D$

If 1, m, n be put = Oit can be seen from the first relation that D = 1A + mB + nC where 1, m, n are integers, now putting Y + D, instead of Y we have $Y_{loc}^{'} = (-1)qX_{loc}q^{-1}$. In the same way D_{loc} and be made to take the form pA + qB + rC where $0 \le p, q, r < 1$. Thus every symmetry relation implies a relation of the type

 $Y = (-1)^{\alpha} Xq^{\alpha}$ for the skeletal lattice, and of the type $Y = (-1)^{\alpha} Xq^{\alpha} + pA + qB + rC$ for a component set, or for the whole system. If in addition the system has no relation of the type $Y = (-1)^{\alpha} Xq^{\alpha} D'$ where q'' = q

the above relations are called the reduced symmetry relations of the skeletal lattice and of the system respectively.

Equivalent Points, Simple and multiple Systems.

A point system possesses in general m distinct reduced symmetry relations, m being always finite or there would be an infinite number of points in each component set. Of these m relations n only will be independent all the others can be derived from these m by combining them in different ways. To any point X there correspond the points X_1, X_1, \ldots, X_m to which it is related by the m relations, also the points $X_p, X_{p,1}, \ldots, X_n$ derived from X by the m relations applied 2, 3, ... k times each the values of k will be explained subsequently, All the points $X_1, X_2, X_3, \ldots, X_m$ belong to the same component set, they are called equivalent points.

If these are all the points in each component set, the point system is called simple. If there are other groups of equivalent points $/Y_r$ $/Z_r$ etc the system is called mmultiple. The groups $/X_r$, $/Y_r^*$ etc may have more but cannot have fewer symmetry elements than fittle system. The group with the

fewest symmetry elements determines the symmetry of the system.

If /X_is such a group the other groups /Y_,/Z_? can be split up into partial groups /Y_,/Y_etc. each with the symmetry of /X and derivable from each other by relations not included in the symmetry of /X_ the whole system is now expressible as: the points X_,Y_?Y_,...,Z_,Z_? and their equivalent points making up accomponent set; and the points corresponding to all these points. The points X_,Y_,Y_,...,Z_,Z_....

may be infinite in number and taken together make up a geometrical figure which is in genefal asymmetrical. For most purposes however it is sufficient to consider simple systems remembering that every point may represent an asymmetrical figure.

CHAPTER III

ROTATIONS

3.3 Symmetry of System and of Skeletal lattice.

It has been shown already that if a system has a symmetry relation $Y=(-1)^{n}qXq^{-1}+D$ the skeletal lattice has the relation $Y=(-1)^{n}qXq^{-1}$. Such relations not involving any constant vector are called rotations. They are in fact representable geometrically by a rotation of the whole system about the axis of q through twice its angle. Further we must have if $Y=(-1)^{n}qXq^{-1}+D$, is the symmetry group of the system that the skeletal lattice possesses the group of rotations $Y=(-1)^{n}qXq^{-1}$. We must therefore examine all the possible classes of groups of rotation that lattices can possess.

.2 Possible Rotations.

To begin with we need only consider the form Y=qXq for since
the relation Y=-X holds for all lattices Y=qXq always implies Y=-qXq correspond
and only those relations of the second kind which to possible relations of the first can exist.

Writing q in the form A where A is a vector and h a scalar the general rotation becomes,

The vector A is called the axis of the rotation.

This relation implies $Y = A^{nh}XA^{-mh}$ where m is an integer.

But $Y = A^{2n}XA^{-2n}$ i.e. Y = X is always a relation of the lattice.

Combining we have $Y = A^{mk+\ell n} X A^{-mk-2n}$

Now mh+En at where e is a finite positive scalar or (X-Y) would not be a finite vector; h must therefore be rational writing h in the form $\frac{2}{k+\frac{m}{n}}$ where k,m,n are integers and n>m then $kh=\frac{2k}{k+\frac{m}{n}}=2-\frac{2m}{k+\frac{m}{n}}$

$$2-kh = \frac{2}{\frac{K^{n}+1}{p}}$$
 where p is an integer > m

and this must be a possible value of the index of A. Continuing the process we must arrive ultimately at a value $\frac{2}{k}$ since the value reduced general rotation now takes the form

Y = A XA X

Such a rotation is called a k fold axis of symmetry because repeated k times it leaves the aspect of the lattice as it was to begin with.

- .5 Possible values of A and k.
- .31 From the conditions of symmetry we have

S.AY E S.AX

S.A(Y-X) = 0

but (Y - X) must be a point of the lattice for all corresponding values of Y and X. This shows that in a plane through any point of the lattice perpendicular to any maxis of symmetry there is a net of points of the lattice.

.32 Further let
$$X_1 = A^{\frac{1}{4}} X A^{\frac{1}{4}}$$

 $X_2 = A^{\frac{1}{4}} X A^{\frac{1}{4}}$
 $X_3 = A^{\frac{1}{4}} X A^{\frac{1}{4}}$
 $X_4 = A^{\frac{1}{4}} X A^{\frac{1}{4}}$

adding SX = A I I, A

this is only possible if $\{X_n = pA\}$ but as the value of the tensor of A does not affect the symmetry relation, and $\{X_n\}$ is a point of the lattice Apan always be chosens a point of the lattice.

Let X_1, X_2, X_3 be three points of the lattice satisfying the conditions S.AX = S.AX = S.AX = 0

$$\mathbf{X}_{1} = \mathbf{A}^{\frac{1}{2}} \mathbf{X} \mathbf{A}^{-\frac{1}{2}} : \mathbf{X}_{1} = \mathbf{A}^{\frac{1}{2}} \mathbf{X} \mathbf{A}^{-\frac{1}{2}}$$

.33

Rational values of p;q;r can always be found such that

$$pX_1 + qX_2 + rX_3 = 0$$

Multiplying throughout by X, and taking scalar products

$$pS.X_{1}X_{2}+qX_{1}^{2}+rS.X_{3}X_{1}=0$$

$$(p+r)X_{2}^{2}\cos\frac{2\pi}{h}+qX_{2}^{2}=0 \quad \text{since } S.X_{1}X_{2}=S.X_{3}X_{3}=X_{2}^{2}\cos\frac{2\pi}{h}$$

$$\cos\frac{2\pi}{h}=\frac{-q}{p+R}$$

see $\frac{2\pi}{K}$ is rational it can only have the values

-1, $-\frac{1}{2}$, 0, $\frac{1}{2}$, 1 corresponding to the values

2, 3, 4, 6, ∞ of k, and these must be the only values that k can have. Excluding the identical relation $k=\infty$

we have the following theorem.

Is any lattice or point system there can only be axes of 2, 3, 40r6 fold symmetry. Such axes are known as diad, triad, tetrad and herad axes respectively The general rotation must now take one of the particular forms

$$k = 2$$

$$= 3$$

$$Y = A^{\frac{1}{2}} X A^{\frac{1}{2}}$$

$$= 4$$

$$Y = A^{\frac{1}{2}} X A^{\frac{1}{2}}$$

$$= 6$$

$$Y = A^{\frac{1}{2}} X A^{-\frac{1}{2}}$$

Combinations of Rotations

a41

We will first establish some trigonometrical formulae connecting angles between axes and their angles of rotation i.e. the angles $\frac{g_W}{K}$

Transform a rotation $Y = \mathbf{A}^{\frac{1}{2}} \mathbf{A}^{\frac{1$

$$\sin\frac{\theta}{r} = \sin\frac{\pi}{h}\sin\phi$$

where ϕ is the angle PAB

Combining the two relations $Y = A^{\frac{1}{4}}XA^{\frac{1}{4}}$ and $Y = B^{\frac{1}{4}}XB^{\frac{1}{4}}$ we have $Y = A^{\frac{1}{4}}B^{\frac{1}{4}}XB^{\frac{1}{4}} = C^{\frac{1}{4}}XC^{\frac{1}{4}}$ where $C^{\frac{1}{4}}=A^{\frac{1}{4}}B^{\frac{1}{4}}$, writing the quaternions in full $(\cos \frac{\pi}{n} + C\sin \frac{\pi}{n}) = (\cos \frac{\pi}{n} + A \sin \frac{\pi}{n})(\cos \frac{\pi}{n} + B \sin \frac{\pi}{n})$

008 # - 008 # 008 # +008 θsin # sin # Where θie the angle A

Consider the two equivalent rotations $Y = A^{\frac{1}{2}}XA^{\frac{1}{2}}$, $Y = B^{\frac{1}{2}}XB^{\frac{1}{2}}$.

Transforming the second by the first gives $Y = B^{\frac{1}{2}}XB^{\frac{1}{2}}XB^{\frac{1}{2}}$.

A rotation 6 may exist that transforms B into A and A into B.

Then

B = C AC and B \cdot C AC. From these we have

B-A = C (A-B)C

The angle between (B-A) and $(A-B) = \int_{a}^{B}$

$$\cos \frac{r_{B}}{m} = \frac{-S(B-A)(A-B)}{S(B-A)S(A-B)}$$

 $= \frac{-1+2\cos\theta-\cos\frac{\pi}{\pi}-\cos2\theta\sin\frac{\pi}{\pi}}{-22+2\cos\theta} \text{ where } \theta \text{ is the angle between A and B.}$

=1-sin' (1+cos)

That is $\sin \frac{\pi}{n} = \sin \frac{\pi}{n} \cos \frac{\theta}{2}$ or $\cos \frac{\theta}{2} = \frac{\sin \frac{\pi}{n}}{\sin \frac{\pi}{n}}$

Giving m and n all allowable values for which m > n we obtain all the possible values of $\cos \frac{h}{2}$ which are shown in the following table

:m-6	: 1	√2 √2	/3	<u>i</u> 2	
:	:	:	. 79.	: :::.	: :
	:;			: . 9	: :
: 2	:	; : :	: : [.]	1	: : :•••

from this we see that

搬机过

- 6 fold axes cannot exist in different directions
- 4 fold axes must be at right angles
- 3 fold axes must intersect at angles of cos for the complementary a angle of cos 14.
- 2 fold axes when equivalent must intersect at angles of $\frac{2\pi}{3}$ $\frac{1}{2}$ $\frac{\pi}{3}$

,5 Classes of Rotation groups; First Sort,

.51

We are now in a position to consider the various classes into which groups of rotations of the first sort may be divided. These collasses will be designated for convenience of reference, by their Schoenflies symbols.

Groups containing one rotation only. General type $Y = A^{\frac{1}{K}} X A^{\frac{1}{K}}$ There are four classes $k = 2 \cdot 3 \cdot 4 \cdot 6$ symbol $C_1 \cdot C_2 \cdot C_3 \cdot C_4 \cdot C_5$

Groups with one k fold and 2 fold axes only.

General type $Y = A^{\frac{1}{2}}XA^{\frac{1}{2}}$ B_1, B_2 ? are equivalent axes. Any two $Y = B_1XB_2^{-1}$ of the axes A? B_1, B_2 B_3 can be taken $Y = B_2XB_2^{-1}$ as the independent rotations of the $Y = B_2XB_2^{-1}$ group.

```
Here again there are four classes:
                                                                                           symbol
                                                                                                                          BeQ D, D
                                                                                       With the conditions S.BC = S.CA = S.AB = 0
                                                  Y = AXA
            Rotations
Q
                                                  Y = BXB
                                                  Y = CXC-
                                                                                                                                                                       S.\overline{ABC} = -1
                                                  Y = At XAt
                                                                                                                                                       S. AB = S. AC = S. BC = 0
D
                                                  Y = BXB
                                                                                                                                                                          Bec
                                                  Y = CXC
                                                  Y = (B+C)X(B+C)
                                                   Y = (B-C) X (B-C)
                                                  Y = A XA F
                                                                                                                                                     $.AB =S.AC =S.AD =0
D,
                                                   Y = BXB
                                                   Y = CXC-
                                                                                                                                                     S.CD = S.DB = S.BC = -1
                                                   X = DXD
                                                                                                                                                                  B = C^{2} = D^{2}
D,
                                                   Y = BXB
                                                                                                                                                                     B+C+D = 0
                                                   Y = CXC
                                                   Y = DXD
                                                                                                                                                               Same asD
                                                   Y = (C+D)X(C+D)
                                                   Y = (D+B) X(D+B)"
                                                    Y = (B+C)X(B+C)-
                 More than one k fold axes (k>2) . There are two classes:
 T with triad and diad axes; O with tetrad, triad and diad axes.
  Both have a set of four triad axes T, T, T, T, T, which are all equival-
  ent and must by 343 and considerations of symmetry fulfil the condit-
  ions ST, T, = - 1 : T, = T, = T, = T, = T, : T, + T, + T, + T, = 0 there, in addition
                  In class T_A^{*} only the three diad axes A,B,C related to T_1, T_2, T_3? T_4
  by the rotations wwritten in their symmetrical form)
      \Delta T_1 - T_2 \Delta = \Delta T_3 - T_1 \Delta = BT_1 - T_3 B = BT_2 - T_2 B = CT_1 - T_2 C = CT_2 - T_3 C = 0
      T^{\frac{1}{2}}B - \partial T^{\frac{1}{2}} = T^{\frac{1}{2}}C - AT^{\frac{1}{2}} = T^{\frac{1}{2}}A - BT^{\frac{1}{2}} = T^{\frac{1}{2}}B - CT^{\frac{1}{2}} = T^{\frac{1}{2}}C + AT^{\frac{1}{2}} = T^{\frac{1}{2}}A + BT^{\frac{1}{2}} = 0 similarly
   for T and T4, from these we find S.BC -S.CA -S.AB - O A -B - C -
   also T_r=A+B+C; T_r=A-B-C; T_r=-A+B-C; T_r=-A-B+C . We have therefore for
                                                     Y = AXA
                Rotations
                                                      Y = BXB'
                                                      Y = (A+B+C) X (A+B+C) Y = (A B C) X (A B C) Y = (A+B C) X (A+B C) Y = (A+B C) X (A+B C) X (A+B C) X (A+B+C) X (A+C) X
```

.53

Class O differs by having A?B,C as tetrad axes and in consequence has four more triad axes whach by virtue of the relations/ $T_3 = A^{\frac{1}{4}}T$, $A^{\frac{1}{4}}$ are the inverses of the original four. Also for the same reasons as D₄ it has three pairs of diad axes of the type B+C or $T_1 - T_2$. Inall there, thirteen rotations any two of which may be chosen as independent if they are of different kinds.

```
Y = A X A 1

Y = B 1 X B 1

Y = C 1 X C 1

Y = (A+B+C) X (A+B+C) 1

Y = (B+C) X (B+C) 1

Y = (B+C) X (B+C) 1

Y = (C+A) X (C+A) 1

Y = (C+A) X (C+A) 1

Y = (A+B) X (A+B) 1

Y = (A+B) X (A+B) 1
```

There are no other classes of rotation groups of the first sort By 343there are no other arrangements of triad and tetrad axes possibly than those of T and O and a lattice can only posses one hexad axis.

The general rotation of the second sort is $\mathbf{Y} = \mathbf{A}^{\frac{p}{k}} \mathbf{I}^{-\frac{p}{k}}$

Combined with another relation of the second sort it gives fise to one of the first sort, so we need only consider classes containing second sort operations only or those formed by combining with one of the classes of the first sort one rotation of the second sort. Further since the effect of combining $Y = A^{\frac{1}{2}}XA^{\frac{1}{2}}$ and $Y = -A^{\frac{1}{2}}XA^{\frac{1}{2}}$ to form $Y = -A^{\frac{1}{2}}XA^{\frac{1}{2}}$ is the same as that of combining $Y = A^{\frac{1}{2}}XA^{\frac{1}{2}}$ and $Y = -X^{\frac{1}{2}}XA^{\frac{1}{2}}$ we need choonsider the combinations of $Y = -XXA^{\frac{1}{2}}$ with classes of the first sort which have no axis in the direction $A = Y = -AXA^{\frac{1}{2}}$ is the only second sort rotation which can be combined in this way because allt the others include a rotation of the first sort.

.61 Second sort operations alone . General type . Y=- $\frac{1}{K}$ IA There are five classes $K=\infty$ 2 3 4 6

Symbol C_L C_S C_{7L} C'_4 C_{3h} C_L Rotations Y = -X This is called a centre of symmetry. C_S " $Y = -AXA^{-1}$ " " a plane of symmetry. C_{3L} " $Y = -A^{\frac{1}{3}}XA^{\frac{1}{3}}$ Y = -X $Y = A^{\frac{1}{3}}XA^{\frac{1}{3}}$ $Y = -A^{\frac{1}{4}}XA^{\frac{1}{3}}$ $Y = -A^{\frac{1}{4}}XA^{\frac{1}{3}}$ $Y = -A^{\frac{1}{3}}XA^{-\frac{1}{3}}$

Except in the case where the axis to which A is perpendicular is a diad axis. We have therefore also to consider the results of combining second class aperat rotations with perpendicular find axes.

```
22
.62
             Combination of YE-X with first sort, and classes
      Ten classes corresponding to C_2 C_3 C_4 C_5 Q D_4 D_4 D_5 T O
                                      \textbf{Symbol} \qquad \textbf{C}_{2k} \ \textbf{C}_{y_\ell} \ \textbf{C}_{dk} \ \textbf{C}_{i,4} \ \textbf{Q}_k \ \textbf{D}_{3\ell} \ \textbf{D}_{dk} \ \textbf{D}_{d_k} \ \textbf{T}_k \ \ \bar{\textbf{U}}_k 
      One of these Cylbelongs also to the last set so that their are really
      only nine classes.
     Czi
             Relations inaddition to those of C.
                                                                    X = -AXA-,
             Conditions as for
     C3,
                                                                  \lambda = V_1 X V_2
\lambda = -X
                                                             C,
     C44
                                                            C,
                                                                    Y = -X
                                                                   YE-AXA"
                                                                    A = - Ve XV.
     Ġ,
                                                            ٥
                                                                   Y=-X
                                                                   Y= -AXA-
                                                                   Y = -ATXAT
     Q,
                                                            Q
                                                                   X-EY
                                                                   Y = -AXA-
                                                                   Y= -BXB-/
                                                                   Y = -CXC
    Dy
                                                           D,
                                                                   Y=-X
Y=-A'XA'
                                                                   Y = -BXB-'
                                                                   Y = -CXC~
                                                                   Y = -DXD-
    D<sub>44</sub>
                                                           D
                                                                   Y = -X
                                                                   YE -AXA-
                                                                  Y = -A+XA-
                                                                   Y = -BXB-
                                                                  Y = - CXC-'
```

5.44

 $Y \equiv (C+D)X(C+D)^{-1}$ $Y \equiv (D+B)X(D+B)^{-1}$ $Y \equiv (B+C)X(B+C)^{-1}$

```
conditions as for
                                                   YE -AXA-'
                                                   Y = -BXB^{-1}
                                                   Y = -CXC^{-1}
                                                   Y = -(A+B+C)X(A+B+C)^{\frac{1}{2}}ETG.
0,
                                               0
                                                    Y= -X
                                                   Y=-AXA-
                                                    Y=-BXB-
                                                    Y= -CXC-'
                                                    Y= -(B+C)X(B+C) ETC.
                                                   Y=-ATXAT ETC.
                                                   Y = -(A+B+C)^{\frac{1}{3}}X(A+B+C)^{-\frac{1}{3}}ETG.
      Combination of Y BIE with rotations of the first sort
                                                    C.
                                                          C
Four classes corresponding to
                                        0,
                                              C,
                                              Csir
                          Symbol
                                        C,
                                                   Car Car
                                                    Y = -BXB"
                                              C.
     Relations inaddition to those of
                                                    Y= -CXC"
                                                    Y = -BXB
C,,
                                              C,
                                                    ¥ = -CXC ~
                                                    Y = -DXD -'
Cir
                                                    Y = -BXB-'
                                                    Y = -CXC-'
                                                    Y = -DXD"
                                                    Y = -(C+D)X(C+D)-
                                                    Y = -(D+B)X(D+B)-'
                                                    Y = - (B+C) X (B+C)-
C<sub>4</sub>,
                                                    Y = -BXB^{-1}
                                                   YY = -CXC-'
                                                    Y = -(B+C)X(B+C)
                                                    Y = - (B-C)X(B-C)
 The only other class of the first sort with no axes perpendicular
 to a! k fold axis (k > 2) is T. From this we have therefore one
                                                        Y= -(B+C)X(B+C)-'
Y= -(B-C)X(B-C)-'
Y= -(C+A)X(C+A)-'
 class T, Relations in addition to Thoseof T
```

THAT BEEF BOOKS IN

Y=X

Y = +C -A)X(C-A)-'
Y = -(A+B)X(A+B)-'

Y= -(A-B)X(A-B)~

Relations in addition to those of T

ŧ

.63

B+C+D =0

.64 Lastly we have to consider the classes which are the result of combining a diad axis Y REBY with with a rotation of the second sort Ym $-\Delta^{\frac{1}{N}}XA$ where S.AB = 0 and k > 2. There are three classes AS $Y = -A^{\frac{1}{2}} X A^{\frac{1}{3}}$ itself possesses a centre of symk = 3 symbol D_/ D_{2/} D3L metry D_must have one and we have already dealt with it. There remain two new classes D, whose rotations are $Y = -A^{\frac{1}{2}}XA^{\frac{1}{2}}$ with the conditions Y = AXA S.AB = S.AC = S.BC = 0 Y = -(B+C) X(B+C)-' RE-CE Y = -(B C)X(B C)-D₃₄ Y = -A'XA" 3.AB = 3.AC = 3.AD = 0 Y = BXB-' S.CD = S.DB = S.BC = -1 Y = CXC-' Y = DXD-B'=c'-n' $\mathbf{Y} = -(\mathbf{C} + \mathbf{D}) \mathbf{X} (\mathbf{C} + \mathbf{D})^{-1}$ $Y = -(D+B)X(D+B)^{-1}$

IN both these cases can be expressed alternatively with rotations $Y = -AXA^{-1}$ etc and $Y = (B+C)X(B+C)^{-1}$ etc. This is as some importance subsequently.

.7

Y = -(B+C)X(B+C)-

We' have now derived all the classes of both sorts into which groups of rotations can be divided. There are thirty two in all, if we include that class with no rotation buy the identity relation Y=X They are divided for reasons that willappear later into five "systems" I. Triclinic system

C, .C. II. Monoclinic system C, ,C, ,C,, III. Orthorhombic system C, D, D, or Q Q, IV. Tetragonal system (a) tetrad axis 1st sort C_4 , C_{4r} , C_{4k} , D_4 , D_{4k} . (b) M: 2nd " C'_{\perp} , $D_{z'}$. V. Rhombohedral system C3 , C3, , C3, , D3 , D3,

VI. Hexagonal system (a) Hexad axis 1st sort C_{ζ} , C_{dA} , $C_{d_{F}}$, D_{ζ} , D_{A} .

(b) " 2nd " C_{3A} , D_{3A} .

VII. Regular system D_{6h} D_{6h} . The classes C_i , C_{2h} , Q_h , D_{4h} , D_{3d} , D_{6h} are called holohedral. Holohedral classes have all the rotations of both sorts that are in the other classes of the same system.

The classes C_1 , Q_1 , D_2 , D_3 , D_4 , D_6 , D_6 , D_8 , $D_$

LATTICES

O Types of symmetrical lattices .

1

We are now in a position to examine the number of types to to one of which any lattice must correspond. The symmetry of any lattice must be that of one of the thirty two classes, but the following considerations show that the choice of these is limited.

- vector perpendicular to A such that no vector B also perpendicular to A exists max making B > B. Then if B, = A BA BA the pairs

 B .B and B .B must be primitive vectors for the net perpendicular to A . Also since B = B B B B and likewise B and B must be diad axes for the net , further A .B .B and -A .B .B are congruent reference systems which are related by a rotation about B so that B must be a diad axis of the maximal trice. From this we have the theorem There are diad axes perpendicular to every triad tetrad, and hexad axis of a lattice.
- .02 Every lattice has a centre of symmetry Y = -I. Combining this with the symmetry axes of the lattice we have the theorem. Perpendicular to every diad, tetrad, and hexad axis of kara lattice there is a plane of symmetry and every triad axis is anaxis of the second sort. From these two theorems we can see that the only classes of symmetry to which lattices can belong are the holohedral classes C_i , C_{IA} , Q_i , D_{IA} , D_{IA} , D_{IA} , D_{IA} , D_{IA} .

C. Let us begin with lattices whose shass of symmetry is that of

C: This is the most general type and the choice of a suitable

reference set is arbitrary so that we can always choose three primitive

vectors a .b .c and write the formula of the lattice

Here and in the subsequent work the small letters a,b,c (d) are used exclusively to denote reference vectors; capitals A,B, being used in the general expressions for axes. The letters l,m,n,c) will always represent integers, while p,q,r,(s) and u,v,w,(t) stand for rational fractions. The rotations of the various lattices are not given here, they are those of the class of symmetry to which the lattice belongs.

Cak

a can here be chosen to be the one diad axis while b and c can be chosen arbitrarily so as to be primitive vectors in the net perpendicular to a. The formula of the lattice is now /pa+qb+re as a,b,c are not necessarily primitive vectors for the lattice. Now if p,q,r is a point of the lattice the rotation Ymaxa gives p,-q,-r, as an equivalent point. By subtraction we find that YMB2p,0,0 and 0,2q,2r must be points of the lattice. But by the choice of the reference set 1,0,0 and 0,m,n are points of the lattice. p,q,r, therefore must have the form $\frac{1}{2}$, $\frac{m}{2}$, When is odd m and n cannot both be even. Now as b and c wre chosen arbitrarily in the first place we can always choose them so that either 1,m,n are always even or so that m is always even and 1 and m both even or both odd. Thus there are two types of lattice whose formulae may be written.

.21 Γ_{m} /la + mb + no .22 Γ_{m}' / $\frac{(1+m)a + (1-m)b + no}{2}$

is Q_h a,b,c are here chosen along the three diad axes. Writing the formula of the mattice in the first place as / la+mb+nc.we can show exactly as in the previous case that the points 2pa, 2pb, 2pb belong to the lattice p,q,r, must have the form $\frac{1}{2}$, $\frac{m}{2}$, $\frac{n}{2}$. Here however as a,b,c are geometrically indistinguishable, there are four types $\Gamma_0, \Gamma_0', \Gamma_0'', \Gamma_0'''$ according as Γ_0 , 1,m,n are always even; Γ_0'' , 1 (say) is always even and mand n are both odd or both even; Γ_0''' two of the numbers are odd and the other is even or they are all even; Γ_0'''' 1,m,n are all odd or all even. The formulae of these are written

.31 Γ_o / la + mb + no With the conditions S.bo = S.ca = S.ab = .32 Γ_o'' / la + $\frac{m+n}{2}b^+$ $\frac{m-n}{2}c$ / $\frac{-1+m+n}{2}a+\frac{1-m+n}{2}b+\frac{1+m-n}{2}c$ / $\frac{m+n}{2}a+\frac{(n+1)b}{2}b+\frac{1+m}{2}c$

- Then either band c are primitives or (b+c) and (b-c) are, but as these are also diad axes band c can always be chosen as primitives. Since a is also a diad axis this is only a special case of Q_k but here there can be no types corresponding to T_k and T_k because when 1 is even mand n must also be even, so that there are only two types: T_k 1, m, n always even; T_k 1, m, n all odd or all even. their formulae are written as before
- .41 T_{ξ} / la + mb + nc. with the conditions S.ab = S.ac = S.bc = 0 .42 T_{ξ}^{\prime} / $-\frac{1 \text{am} + n}{2}$ a + $\frac{1 - m + N}{2}$ b + $\frac{1 + m - n}{2}$ c : $b = c^{\xi}$

.5 0_h a,b,c are chosen along the three tetrad axes, and since all three are diad axes as well, the case is similar tothat of Q_k except that in this case symmetry makes \mathcal{T}' the same as \mathcal{T}'' so that in this class there are three types only

.51
$$\Gamma_r$$
 / la + mb + nc . With the conditions
.52 Γ_r / $\frac{m+n}{2}a + \frac{n+1}{2}b + \frac{1+m}{2}c$ S.bc = S.ca = S.ab = 0
.53 Γ_r / $\frac{-1+m+n}{2}a + \frac{1-m+n}{2}b + \frac{1+m-n}{2}c$

- .6 D₃₄ In this and the succeeding class four reference vectors will be chosen, this is not strictly necessary but it exhibits the symmetry of the lattices. Whenever four vectors are taken the linear relation between them of the type pA+qB+rC+sD=0 imposes a relation of the type tp+uq+vr+ws = 0 upon the coordinates of any point If the coordinates satisfy such a relation there can be no ambiguity about them .
 - a is taken along the triad axis, b, c, d along the diad axes perpendicular to it. The formulae of the lattices can then be written ζ / Pa+qb+rc4sd with the condition q+r+s=0. In the net /qb+rc+sd any pair of b, c, d are primitives. Any point of the net is mb+nc but to satisfy the condition we must add t(a+b+c)=0 so that m+t+n+t+t=0, 3t must be an integer. The most symmetrical expression that satisfies these conditions for points in the net is

$$\frac{21-m-n}{3}b + \frac{-1+2m-n}{3}c + \frac{-1-m+2n}{3}d$$

with the condition 1+m+n=0 Now by the rotation about a there are the three corresponding points of the lattice p,q,r,s; p,s,q,r and p,r,s,q hence we must have the point 3p,(q+s+r),(r+q+s),(s+r+q) that is the point 3p,0,0,0. Therefore 3p=1 quarteger also by rotation about b there are the corresponding points

p,q,r,s, and -p,q,r,s; hence the point 0, 2q, (r+s),(s+r) and similarly the points 0,(s+q),2r,(q+s) and 0,(q+r),(r+q),2s and since these must be points of the net /(21-m-n)b/3 + q,r,s must be of the form 1/3,m/3,n/3. Now if since p+q+r+s0 0 (2m-n-o)/3,(-m+2n-o)/3,(-m-n+2o)/3 we may write q,r,s either as intiputs or aw (m-n)/3,(n-1)/3,(1-m)/3. This leads to two lattices: $\sqrt{\frac{1}{4}}$ written

- /la+(2m-n)-o)b/3+(-m+2n-o)c/3+9-m-n+2o)d/3

 For 1 must be an integer as the remainder of the expression is the formula of the net 1=0; and Γ_{rh} written
- .62 /(1+m+n)a/3+(m-n)b/3+(n-1)c/3+(1-m)d/3
- .7 D_{6k} Every lattice with a hexad axis also has a triad oneso that the only type of lattice that can correspond to n_k must be one of those corresponding to n_k namely Γ_k and Γ_k . Now in the class $D_{\ell k}$ there are corresponding points p,q,r,s and -p,q,r,s; and hence the point 2p,0,0,0. p must be of the form 1/2 but p cannot at the same time be of the form 1/3 unless P is an integer, and this is only thee case for Γ_k so that there as only one type of hexad latti
- .8 This completes the number of possible lattices. There are fourteen in all and every lattice can be reduced to one of these.

CHAPTER V.

GENERAL SYMMETRY RELATIONS

O Possible forms of the General Symmetry relation.

Returning to the general symmetry relation which we may write $X = (-1)^{\frac{1}{4}} X A^{\frac{1}{4}} + C$ Where $x = 2 \cdot 3 \cdot 4$ or 6

we are now in a position to examine the possible values of the constant. vector C and their significance.

.1 Sorew and Rotation Axes.

Consider the the most general relation of the first sort written in the form $Y = a^{\frac{1}{K}} Xa^{\frac{1}{K}} + ua + vb + wc$ where a, b, c are primitive vectors of the skeletal lattice. If the origin is on the axis a it can only be related to the points pa and consequently v = w = 0 and the relation takes the form

Y= a I Ia +ua

Repeating this k times we obtain

Y = X + kua

whas one of the values $\frac{n}{k}$; but u must also have the value $m! + \frac{n}{k}$ so that the value of n may always be made to lie between such limits as (i) 0 < n < k or (ii) $-\frac{k}{2} < 0 < \frac{k}{2}$

As it is always possible to chose one of the primitive vectors along any axis of the system the same argument applies to all axes, and in general if if so that we may write the general relation of the first sort in the form

 $Y \equiv (pa+qb+ro)^{\frac{1}{K}} I(pa+qb+ro)^{\frac{1}{K}} H(pa+qb+ro) + ua+vb+wc$ where app are the reference vectors of one of the 14 lattices h is an integer and S.(pa+qb+ro)(ua+vb+wc)=0

- when h is not 0 such a relation is called a screw; if h=0 it is called as before a rotation. Consider the two screws $Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + \frac{h}{k} a$ and $Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + \frac{h}{k} a$ where $h < \frac{k}{2}$. The second may be writte in the inverse form $Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + \frac{h}{k} a$ which shows that it differs from th first only in the sense of its rotation, if the sense of one is that a right handed screw the second is left handed, and vice versa. If however k=2 or 2h=k right and left handed screws are indistinguiable.
- When h is a factor of k the screw reduces to $Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + \frac{a}{k}$, where kh = k Repeating k times we have $Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + a$, ther is a rotation $Y = a X a^{\frac{1}{k}}$.

The possible types of screws and rotations are given in the table of they are expressed as if the axis passed through the origin and with a primitive vector a as axis but this is only for convenience esake.

.13 Types of screws and rotations.

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Y = a^{\frac{1}{K}} X a^{\frac{1}{K}} + \frac{h}{K} a
General form
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Particular forms

k-6

.2 Axes not throught the origin

We may now write the general relation of symmetry of the first sort in the form $Y = A^{\frac{1}{K}}XA^{\frac{1}{k}} + pA + B$ where S.AB=0 Let us change the origin to a point C where S.AC=0 If Xand Y are the new values of X and Y then X = X + C; Y = Y + C and the relation becomes $Y + C = A^{\frac{1}{K}}(X + C)A^{\frac{1}{K}} + pA + B$

 $Y = A^{\frac{1}{K}}XA^{\frac{1}{K}} + pAA^{\frac{1}{K}}CA^{\frac{1}{K}} - 0 + B$

The axis passes throughthe new origin if

This equation gives the the position of any screw or rotation axis in terms of the constants of its symmetry relations.

An important particular case is when Ais the reference vector a, and B takes the form vb+wc S'ba=S.ca=0

If also a ba fb+gc a ca fp+go the equation for a point on the axi takes the form x(f,b+g,c)+y(f,b+g,c)-xb-yc+vb+wc=0which gives for pand y (1-f,)x-fy=wv-g, x+(1-g,)y=w

3 Relations of the second sort

As before we may write the general relation of the second sort

in the form

$$Y = -A XA + pA + B \qquad \text{where S.AB} = 0$$

Transferring the origin to the point $\frac{PA}{2}$ + B' S.AB'=0 we have $Y = -A^{\frac{1}{K}} X A^{\frac{1}{K}} - A^{\frac{1}{K}} B A^{\frac{1}{K}} B + B$

and if B is chosen to satisfy $A^{\frac{1}{K}}BA^{\frac{1}{K}}+B-B=0$ this reduces to $Y=-A^{\frac{1}{K}}XA^{\frac{1}{K}}$

Thus the general relation of the second sort, except in the particular reduces to a rotation of the second sort.

case k=2, whose centre is in general not the origin. In particular the general inversion Y=-X+B is a centre of symmetry at the point B

31 Reflections and glide planes

In the case k=2 the equation for the centre becomes $ABA^{-} + B = 0$

$$-B'_{+}B'_{+}B = 0$$

From this equation we see that B-coland that in general the equation cannot be reduced any further than

This relation repeated once gives

B must take the form $\frac{1}{2}(pa+qb+ro)$ where pa+qb+ro is a vector of the skeletal lattice, this may always be reduced to one of the forms $0,0,0;\frac{1}{2},0,0$ etc $;\frac{1}{2},\frac{1}{2},0$ etc $;\frac{1}{2},\frac{1}{2},\frac{1}{2}$; or if p,q,r are of the form $\frac{1}{2}\frac{m}{2}\frac{n}{2}$ or $\frac{1}{3}\frac{m}{3}\frac{n}{3}$, to $\frac{1}{4},0,0$ etc or $\frac{1}{6},0$, 0 etc If the plane can be reduced to the form Ym-AXA+::pAwhere S.AB=0 it is called a plane reflection; if it reduces to the form Ym-AXA+pA+B it is called a gliding-reflection; in either case the plane passes through the point $\frac{1}{2}$ pA.

4 Parameters of the general symmetry relation.

If the general relation be written in the form $Y \equiv (-1)^{Y} A^{\frac{A}{K}} X A^{\frac{1}{K}} + ua + vb + wc$

u, v, w are called the parameters of the relation, they fix the type of the relation when the axis and rotation are given. The origin can always be chosen either to be on the axis of rotation or in the plane of rotation, which allows u, v, w to be given any desired values subject to certain restrictions; one for an axis, two for a plane, none for a centre of symmetry.

The symmetry of a point system is completely determined when the rotations and parameters of: its symmetry relations are known

i.e. if / x = (1) A X A + ua + vb + wo are known

shoice of the same origin being taken for all of them . A change of origin will give different values for the parameters but there are some invariance relations between them. Two particular cases are of special importance

.41 If three of the relations are of the form

Here it is easily seen that change of origin does not alter the values of the three quantities $u_{\underline{c}}u_{\underline{s}}$, $v_{\underline{s}}v_{\underline{s}}$, $w_{\underline{c}}v_{\underline{s}}$; and that any three parameters, one chosen from each of the pairs $u_{\underline{s}},u_{\underline{s}};v_{\underline{s}},v_{\underline{s}};v_{\underline{s}};v_{\underline{s}},v_{\underline{s}};v_{\underline{s}};v_{\underline{s}};v_{\underline{s}},v_{\underline{s}};v_{\underline{s$

If the class of symmetry is hemimorphic and it has relations

Y = a k x a k + ua + vb + wc

Y = -b x b' + ua + vb + wc

Y = -c x c' + ua + vb + wc

here only $v_i - v_j$ and $w_i - w_j$ are unaltered by change of origin and only two of v_i , v_j ; w_i , can be given any desired value.

.5 Relations between parameters

In general the set of parameters in any class of symmetry all are not, independent, they are connected by relations and can can be determined when some of them; usually one, two or three are known.

As these can only have some few fractional values the number of of types of symmetry in any class is always finite. It is the purpose chapter of the next section to derive all these types, but it is first necessary

to obtain in their mast general form some of the relations connecting the parameters of different symmetry relations.

Relations with the same rotation

1 Parallel axes

Consider the symmetry relations

$$Y = A^{\frac{1}{k}} X A^{\frac{1}{k}} + hA/k+B$$
 Where S.AB = S.AB = O
 $Y = A^{\frac{1}{k}} X A^{\frac{1}{k}} + hA/k+B'$

Subtracting we have $Y = Y = (\underline{h'-h})A + B'-B$. $(\underline{h-h})A + B'-B$ must be a point of the skeletal lattice. In general $A = pa \cdot qb + rc$ B = ua + vb + wc B' = ua + vb + wc

with the conditions $\angle upa^2 + \angle (vr+wq)S.bc = 0$ $\angle upa^4 + \angle (vr+wq)S.bc = 0$

then if pa+qb+ro represents a vector of the lattice, we have $\frac{h'-h}{k}(pa+qb+ro)+(u'-u)a+(v'-v)b\cdot(w'-w)c=pa+qb+ro$

which gives the three conditions

$$\frac{h'-h}{k}p_{\sigma}+u'-u=p ; \frac{h'-h}{k}q_{\sigma}+v'-v=q ; \frac{h'-h}{k}r_{\sigma}+w'-w=r .$$

An important particular case n=1; v=0; v=0: S.ab=S.ac=0 $\frac{h-h}{h}=p ; v-v=q ; w-w=r;$

If p,q,r take the form 1,m,n h'-h=k1; all parallel screw axes must have the same pitch.

.62 Parallel planes

Consider the planes

 $Y \equiv -AXA^T + ua + vb + wc$; $Y \equiv -AXA^T + ub + vb + wc$. Subtracting and equating to a vector of the lattice.we obtain

In the particular case where A = a and p,q,r. are l,m,n we see that parallel planes are all reflection or all glide planes and that they are placed at distances $\frac{1}{2}$ l apart.

.62 Centres of symmetry

Consider the two centres Y=-X +ua+vb+wc; Y=-X+ua+vb+wc

subtracting and equating to a vector of the lattice we obtain

there are centres of symmetry at all the points

7 Relations with different rotations

71 Perpendicular axes

Consider the relations

$$Y = a^{\frac{1}{k}} X a^{-\frac{1}{k}} + ha/k$$

Where Sab = S.ac = 0

$$Y = (qb+rc)X(qb+rc)^2 +ua+vb+wc$$

Transforming the first by the second we obtain

$$Y = a^{\frac{1}{2}} X a^{\frac{1}{2}} + ha/k = a^{\frac{1}{2}} (vb+wc)a^{\frac{1}{2}} + vb+wc.$$

subtracting the original relation and equating to a point of the latti

And if $a^{\frac{1}{k}}ba^{\frac{1}{k}}=fb+go$; $a^{\frac{1}{k}}ca^{\frac{1}{k}}fb+go$ we have

.72 Axis and parallel plane

Consider the relations

$$Y = a^{\frac{1}{k}} X a^{\frac{1}{k}} + ha/k$$

transforming the first by the second we obtain

$$Y = a^{\frac{1}{2}} X a^{\frac{1}{4}} - ha/k - a^{\frac{1}{4}} (Vb + Wc) a^{\frac{1}{4}} 4Vb + Wc$$

This is seen to be an screw of opposite pitch. Subtracting from the original relation and equating we haven

$$2ha/k+a^{\frac{1}{k}}(vb+wc)a^{\frac{1}{k}}-vb-wc=pa+qb+rc$$

If as before $a^{\frac{1}{k}}ba^{\frac{1}{k}}=fb+gc$; $a^{\frac{1}{k}}ca^{\frac{1}{k}}fb+gc$ we have 2h=kp; v(f-1)+wf=q; vg+w(g-1)=r.

Axis and Centre of Symmetry.

Consider the relations

$$Y = a^{\frac{1}{k}} X a^{-\frac{k}{k}} + ha/k + vb + wc$$
 where S.ab = S.ac = 0

Y = -X + ua + vb + wc

transforming the first by the second we obtain

$$Y = a^{\frac{e}{k}} X a^{\frac{e}{k}} - ha/k - a^{\frac{e}{k}} (\psi b + \psi c) a^{-\frac{e}{k}} (\psi - \psi) b + (\psi - \psi) c$$

a screw of opposite pitch . subtracting and equating as before

2ha/k+(2v,-v,)b+kw,-w,)c +ak(vb+wc)ak=pa+qb+rc

as above this gives

Spere

2h = kp; $2v_{+}(g_{-1})v_{+}v_{+} = q$; $2w_{+}g_{-1}v_{+} = r$

In this and in the previous case if p is of the form 1 , h $\frac{1}{2}$ k

CHAPTER VI

TYPES OF POINT SYSTEMS

8.0 We are now in a position to to derive the possible types of symmetry of point systems in three dimensions. The plan adopted in the work is as follows.

The symmetry relations of every class are given in their general form. Where, however, any class is derived from another by the addition of symmetry relations, only these relations are given. The conditions connecting the parameters are then found, the origin is chosen and parameters the possible reduced values of sugh, as are chosen to be independent determined. Corresponding to each permutation of these there is a type of symmetry but some of these types may be shown to be geometrially indistinguishable, and will not count as separate types. In general there are several lattices which include any class of symmetry. The types of symmetry corresponding to these lattices will be derived in turn. The lattice whose formula may be written /la+mb+nc where a,b,c are axes of symmetry is dealt with first, to every type of symmetry which it gives rise to there corresponds one for the other lattices of the same class, but here they are not all distinct.

The types are designated by their Schoenflies symbols even when' the order of their derivation would suggest different notation.

In some cases the position and nature of axes and planes are given but these can always be obtained by from the parameters.

The formulae of the various types of symmetry are reserved for a later chapter.

.1 Triclinic Types

Two classes C_i and C_i one lattice T_i

- .11 C, only the identity relation Y= X+ua+vb+wo u,v,w always reducible to 0,0,0 . only one type C
- .12 C_i only the centre Y= -X+ua+vb+wc u.v.w always reducible to 0,0,0 only one type C
- Monoclinic Types . 2

Three classes C_2 , C_3 , C_4 . Two lattices Γ_n and Γ_n^{\prime} .

.21 C_z the axis $Y = aXa^{-1} + ua + vb + wc$ The origin can always be chosen to make v=w=0 By 5.1u=0 or $\frac{1}{2}$ 1561 shows that for l_m^n u=0 and $u=\frac{1}{2}$ give distinct types but that for $\int_{m}^{n} u = 0$ implies $u = \frac{1}{2}$ so that there is only one type. In all there are the three types

 C_z skeletal lattice T_z , parameters 0.0.0

C,

Ľ, 0.0.0, and \(\frac{1}{2}.0.0.\)

C The plane Y -aXa +ua+vb+wc The origin can always be chosen to . 22 make μ 0 . v and w can have the values 0 or $\frac{1}{2}$. In band c have been chosen arbitrarily so that the values for v.w $\frac{1}{2}$, 0; 0, $\frac{1}{2}$; $\frac{1}{2}$, $\frac{1}{2}$ are geometrically indistinguishable so that there are only two distinct types. In by 569 the values 0.0 imply \$2.0 but there are still two. '7 types since b and c are no longer arbitrary, and the values $0,\frac{1}{2};\frac{1}{2},\frac{1}{2}$ are distinct from the former pair. In all th ere are the four types

 C_c skeletal lattice Γ_a , parameters 0,0,0

" 0,0,0 and 0,≸,0

 $0,0,\frac{1}{2}$ and $0,\frac{1}{2},\frac{1}{2}$

.23 Czi Derived from Cz by the addition of the centre

(u = 0

Y=-X+ua+vb+wc The origin can still be chosen so that, By 57we have for Γ_m 2v=1; 2w=m; and for Γ_m $2u=\frac{1+m}{2}$; $2v=\frac{1-m}{2}$; 2w=n but since u cannot= $\frac{1}{4}$ these both give the same possible values for the parameters namely 0,0,0; $0,\frac{1}{2},0$; $0.0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$. For Γ_m the last three are geometrically indistinguishable, for Γ_m the first two and the last two imply each other. In all there are six types

.3 Orthorhombic Types.

Three classes Q, Q, Q, ; four lattices

.31 Q Three axes Y =aXa +ua+vb+wc

 $Y = bXb^{-1} + ua + vb + wa$

Y = cXo"+ua+vb+wo

Combining the three we obtain Yzaboloba + (u+u-u)a+(v-v-v)b+(w-w+w)c

and since Uabe=-1 we have for
$$\Gamma_{r}$$
 Γ_{r} Γ_{r}

we can always choose the origin to make $u_3 = v_1 = v_2 = 0$ u_1, v_2, v_3 , can take the values Oor $\frac{1}{8}$; here a, b, c are geometrically indistinguishable this leads to four types for Γ_0 , for Γ_0 these reduce

to two since the values 0,0,0 for u_1,v_2,w_3 , implies the values $0,\frac{1}{2},\frac{1}{2}$ and the values $\frac{\pi}{2}$,0,0 implies $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; for Γ all the types reduce to one; for Γ there are again two types 0,0,0 implying $\frac{1}{2},\frac{1}{2},\frac{1}{2}$, and $\frac{1}{2},0,0$ $0,\frac{1}{2},\frac{1}{2}$, so that there are altogether nine types.

Q' a)	celetal	lattic	≜ T, ,	parameters	0,0,0 0 0 0 0 0 0			
ą²		•	Γ,	•	₹ 0 0 0 0 0 1 0 0			
Q 3	•	W	Γ,		0 ±00 0 ± ± 0 0 ±			
Q ⁴		.	<i>T</i> ;	. •				
Q	■ ************************************	ুক্ত ভিচ ব	" "	₩	0 0 0 0	nd O		
Q		* •	ŗ'	•	1 0 0 0 0 0 1 0 0	# 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	and the second s	
Q ⁷	•	•	Γ,"		0 0 0 0 0 0 0 0 0	0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
. 5g			Ţ,***	•	0 0 0 0	and 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
Q,	•	10	T,"	•		" 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1		

From these parameters we can see that

Q'has three intersecting diad axes; Q has one diad screw meeting both of two non intersecting diad axes; Q has one diad axis passing through rectangles the centres of the squares formed by two intersecting diad screws; Q has three non intersecting diad screws; Q is a combination of Q and Q

44

Q'of Q'and Q; Q'combines all the types 2.Q, 2,Q'; Q combines Q'and Q' Q'. Q'and Q'.

.32 C20 An axis and two planes

Combining the three we obtain Ymaboloba + (u,+u,+u,)a+(v,-v,+v,)b+(w,+w,-w,)c and since Uabc = -1 we have ; for Γ_{ϵ}

we can always choose the origin to make $\mathbf{w}_{j} = \mathbf{w}_{j} = 0$

 $\mathbf{u}_{_{2}},\mathbf{u}_{_{3}},\mathbf{w}_{_{2}},\mathbf{v}_{_{5}};$ can take the values 0 or $\frac{1}{8}$. For Γ permutations of these lead to 16 types but since b and c are indistinguishable 6 pairs of t these types are likewise, leaving only 10 distinct types . For $\Gamma_{\!\!o}^{\prime\prime}$ as ab and c are no longer indistinguishable there are two divisions according as we write \overline{L} as $/1a + \frac{m+n}{2}b + \frac{m-n}{2}c$ or as $\sqrt[n]{\frac{1+n}{2}a + mb + \frac{1-n}{2}c}$. In each of these divisions several sets of types corresponding to the 10 above imply each other which reduces the number to 3 in the first and 4 in the second division. For \mathcal{L}'' the number is reduced to two and for \mathcal{L}'' three types. In all there are 22 types which are set forth, with their parameters in the following table.

								-			
	atti	οο Γ _σ , γ	parameters	u 0 0	# 0 0 0	W 0 0 0		e e		्र स	
C _{2,p}		• ·	, ***			000					
C _{2,r}	#	•	•	0	0 0	0 0 0					
9 4 c 7 c 7 c 7 c 7 c 7 c 7 c 7 c 7 c 7 c	•		•	0	Olforia	000					
			•	1 1 1 0	0-10-10	0					
Car	•	. 4	#		000	0					
C _{£r}	•	•			Q 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2						
C	•	ij	•		0						
	*,	*	•	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	01212	012					
C2+	Ħ	ii			0 to to				٠		
C _{2,r} "	•	r,	•	0 0 0		000	and	000	10 to 12	-for-for-for	
C ₂ r	•	n .		18120	0 0	000	17 17	1 1 1 0			
c _{1,-}	•		•	O-late		000	17 17			- to-to-to	•:

```
C lattice P parameters
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0 0 0 " \frac{1}{2} 0 \frac{1}{2}
                            1,0
                                                                                                0 0 1
0 0 0
2 0 0 1
2 0 0 1
                                                                          0 0
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11
                            7,
                                                                                                0 0 0
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                                                                                         #
#
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01-21-20
01-20-20
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1 1 0
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0 0 0
                                                                                                  0 \frac{1}{3} \frac{1}{3} \text{ and } \frac{1}{3} \text{ 0 } \frac{1}{3} \text{ and } \frac{1}{2}
                             17"
                              T, *
                                                                      0 0 0
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                               r,*
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0 0 0
 C21
                                                                            0 0
0 0
0 0
                                                                                                  000
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  Czr
                                 1,"
                                                                                                  0 0 0
0 2 0
0 2 0
                                                                                           17
17
```

.33 Q Derived from Q by the addition of the centre of symmetry Ye = X+ua+vb+wo

By 5.73we have the possible values of u.v.w are $0,0,0;\frac{1}{2},0,0;0,\frac{1}{2},0;0,0,\frac{1}{2};$ Except in types derived from Q_1 , $0,\frac{1}{2},\frac{1}{2};\frac{1}{2},0,\frac{1}{2};\frac{1}{2},\frac{1}{2},0;\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},0,0,0,0,\frac{1}{2},\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},0,0,0,0,0,\frac{1}{2},\frac{1}{2}$ give rise to indistinguishable types leaving only two.

For Q and Q by 563.0,0,0 implies $0, \frac{1}{2}, \frac{1}{6}$; $\frac{1}{8}, 0, 0$ $\frac{1}{2}, \frac{1}{2}$; $0, \frac{1}{6}, 0$ 0,0, $\frac{1}{8}$ and $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{6}$ also in Q 0,0,0 & $\frac{1}{2}, 0, 0$ and $0, \frac{1}{2}, 0$ & $\frac{1}{2}, \frac{1}{2}, 0$ give rise to indistinguishable types but they do not do so in Q so that four types correspond to the farmer and only two to the former.

For 2^{i} and 2^{i} by 5630.0,0 implies $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}$,0.0 $0, \frac{1}{2}, \frac{1}{2}$; etc and as the last three give rise to indistinguishable types there are only two types corresponding to each of 2^{i} and 2^{i} .

Inall there are 28 types

Q'	lattice	1%	derived	from	q' 1	parameters	0	0	0
of the s	#1	•	17		Q'	Ħ	눑	ŧ	1
Q ³	n	11	17	11	ď,	Q	1	0	0
24		4	. 11	*	Q'	17	0	1	1
Q5	*	4		#	Q*	**	0	0	0
Q,			•	Ħ	q	# .	Ì	ì	ł
		**		**	Q*	ч	0	主	0
Q, 8	77	. 4	*	Ж	Q*		0	0	22

Q	lattice	T, der	ived	from	Q ³ para	meters	0 0	0	
	=	n	n .	**	3 3	R	1 2	1	
Q,	*	h	n	Ħ	2³	*	1 0	0	
Q,n	Ħ	11	Ħ	**	૱ ³	•	o į	0	
Q13		4	n		ą³	n ,	0 }	1	
Q'	**	h	n	**	Q^3	n	1 1	0	
Q	**	*	n	*	Q*	*	0 (0	
$\mathbf{q}_{\mathbf{k}}^{R}$	**				Q.	m	1	量	
Q'7	11	Γ,'	#	Ħ	Q ^{5°}	**	0 (0	
Q's	**	7	tt	Ħ	Q ⁵ .	*	1 2	1 2	
Q.	*	• .	Ħ	w		97.5 11	Ģ (o o	
Q;	# . #	- A	17	11 11	a, a,	n	0 1	0 1	
Q,		•	**	11	2	•	1	0]	
Q.	3 W	r,"	n	11	2"	, n	0	0 0	
Q	•	ħ	Ħ	*	Q ⁷	n ·	1	1 1	
Q,15		1, "	п	**	Q ^{\$}	п	-	0 0	
Q.		•	m		Q.	n	l E	0 0	
STEAT OF STEAT OF STATE	, n	4	71 F S	**	Q [†]	Ħ .	0	0 0	
o ^z i	, ₁₁		н	n	۵1	Ħ	ļ	0.0	

Tetragonal Typos

Seven classes C_4 , C_4' , C_{4h} , D_4 , D_4' , C_{4s} , D_{4h} . Two lattices T_c and T_c' . Y= atXat+ua+vb+wo. The origin can always be chosen to C The axis make v = w = 0, u can have the values $0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ (the relations they represent are called tetrad axis, right, neutral, and left tetradscrews respectively) By 56 we have for $\Gamma u = 1$ for $\Gamma u = \frac{1}{2}$ so that for Γ there are given by 5.2, here $f_i = g_i = 0$ $g_i = 1$ $f_i = -1$ so that the coordinates of a point on the axis are given by x+y=v; x-y=w for T_{+} this gives $x = \frac{M+n}{2}$ $y = \frac{m-n}{2}$; for $\frac{n}{2}$ $x = \frac{1}{2}$ m but here if m and n are both odd or even the pitch of the axis differs by 1 from that which passes through a point where one is odd and the other even. The tetrad axis implies the diad axis YmaXa + 2ua and we have from 5.2 these must pass through the points $\frac{1}{2}m$, $\frac{1}{6}n$ for $\frac{1}{6}$ and $\frac{m+n}{4}$, $\frac{m-n}{4}$ for $\frac{1}{6}$; being all of the same kind in the first case and alternately rotation or screw axes in the second In all there are six types

 .42 C_4' the axis $Y_E = a^{\frac{1}{2}} X a^{\frac{1}{2}} + u a + v b + w c$. The origin can always be chosen to make u = v = w = 0 so that there are only two types one derived from Γ_4' and one from Γ_4' . By subtracting $Y_E = a^{\frac{1}{2}} X a^{\frac{1}{2}} w c$ have u, v, w = 1, m, n for Γ_4' and $\frac{1 + m + n}{2}$, $\frac{1 + m - n}{2}$ for Γ_4' . By 52this shows that th centres of the set of alternating tetragonal axes are at the points $\frac{1}{2}, \frac{m + n}{2}$ in the first case and $\frac{-1 + m + n}{2}$, $\frac{1}{2}$, $\frac{m - n}{2}$ in the second.

There are two types

$$C'_4$$
 lattice T'_t parameters 0 0 0 C'_4 = T'_t u 0 0 0 and $\frac{1}{2}$ $\frac{1}{2}$

.43 C Derived from C by the addition of the centre of symmetry

Y=-X:+ua+vb+wc The origin gan be chosen to make u=0 Since by S centre of symmetry trans forms right into left handed screws types of this class can only be derived from the types C_q' , C_q' ,

we have also the conditions: for
$$\sqrt[n]{r}$$

$$2n_{r} = 1$$

$$-1 + m + n$$

$$2$$

$$v_{r} + w_{r} = m$$

$$v_{r} - w_{r} = n$$

$$\frac{1 + m - n}{2}$$

w and w may have the values 0,0 or $\frac{1}{2},\frac{1}{2}$ but for C_{ν}^{f} since u is 0 or $\frac{1}{2}$ w, w can only be 0,0 while for C since u is $\frac{1}{4}$ or $\frac{3}{4}$, w, w can only be $\frac{1}{2},\frac{1}{2}$. There are in all six types.

The parameters are connected by several conditions

Transforming 2 by 1 we obtain Y = cXc + (2u+u)a-wb+vp but this may be

the same as 3 and we have u=u+2u; v=-w; w=v.

similarly for 4 and 5 u_=u-2u;v=w;;w=-v

 $u_3 + u_1$, $u_2 + u_3$, $u_4 + u_4$, $u_5 + u_5$, $u_5 + u_6$, $u_5 + u_7$, $u_7 + u_8$. The equivalent parameters u_1, v_3, w_3 and $u_7 + u_8$, $u_7 + u_8$, $u_8 + u_8$

by Awe have for $\sqrt[r]{v} = \frac{m+n}{2}$; $w = \frac{m-n}{2}$ for $\sqrt[r]{v} = \frac{1}{2}$; $w = \frac{m-n}{2}$ but by the values 0,0,0 for u,v,w, imply the values $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ so that these can only give rise to one case. There corresponds man types of this class to each of types types C_4', C_4', C_4', C_4' , and one to the almost C_4', C_4' ; making 10 in all

45 Du three axes and two planes

 $Y = bXb + ua + v_b + w_c$ $Y = cXc + ua + v_b + w_c$

Y = -(b+c)X(b+c) + na+vb+wcY = -(b-c)X(b-c) + ua+vb+wc

The relations of this class can also be written in aform where diad axes and planes change places each of these ways give rise to distinct types; it is more convenient however to consider them derived from the above relations with skeletal lattices Γ_t , Γ_t written $\ln \frac{m+n}{2} + \frac{m-n}{2}$ and Γ_t written $\ln \frac{m+n}{2} + \frac{m+1}{2} +$

As in D we obtain the conditions $u_i = u_i$; $v_i = w_i$; $w_i = -v_i$, $u_i = u_i$; $v_i = v_i$; $v_i = v_i$

Combining 1,2,3,4 we have: for
$$\Gamma_{1}$$
 Γ_{2} Γ_{3} Γ_{4} Γ_{5} Γ_{5}

As in D_{ij} equivalent parameters u, v, w and u, v+1, w represent different kinds of plane. The actual arrangement of axes and planes can be seen by considering the arrangement in the corresponding types of Q and C.

By 5.71 we have: for
$$T_r$$
 $T_r^{'}$ $T_r^{'}$ $T_r^{'}$ $T_r^{''}$ $T_r^{''$

and by u = 1

For Γ_t Γ_t since u_t , v_t , can have the values $0, \frac{1}{2}$ there are four types each for Γ_t the values 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}$, and $\frac{1}{2}, 0$ imply each other so that there are only two, for $\Gamma_t^{1/4}$ so do 0, 0 and $0, \frac{1}{2}$; $\frac{1}{2}, 0$ and $\frac{1}{2}, \frac{1}{2}$ so that again there are only two.

In all there are twelve types (only the parameters $u_i v_i w_i$ are given) $u_i v_i w_i$

D. 1	atti	se f cor	respor	nding to	o c p	rameters	1 0 0 and	1 1 1 1
D,7	. •	•			Q C		0 0 0	0 1 1
D.*		u j	•	er er	Q 0/1	¥ŧ	1 0 0 1 1 1 2 3 2	草草草
D,"	•	Te'	•		Se. C.	¥	0 0 0	
D'A	*		1	e e e e e e e e e e e e e e e e e e e	q co	H	1 0 0 1 0 0	0 1 1 0 2 2
D.	•	T.	, #		Q' Cto	*	000	0 1 2 2
D.			*		Q 020		$\frac{1}{2}$ 0 0 $\frac{1}{2}$ 0 0	

46 C one axis and four planes

 $Y = a^{2} X a^{2} + ua$ $Y = -bXb^{-} + ua + yb + wa$ $Y = -cXa^{-} + ua + yb + wa$ $Y = -(b + c)X(b + c)^{-} + ua + yb + wa$ $Y = -(b - c)X(b - c)^{-} + ua + yb + wa$

Tx As in D we have the conditions $u_1 = u_1$; $v_2 = -u_1$; $w_3 = v_3$ $u_2 = u_3$; $v_3 = u_3$; $v_4 = v_3$

For T_i since u can only have the values $0, \frac{1}{2}$ and v_i, w_i can only have 0, 0 or $\frac{1}{22}$ there are 8 types. For T_i can have the values $0, \frac{1}{2}$ but 0 implies $\frac{1}{2}$ and $\frac{1}{2}$, further, in the first case the value of v_i , v_i are limited to 0?0 and $\frac{1}{2}$, $\frac{1}{2}$ and these imply each other; while in in the second the values are limited to $\frac{1}{2}$, 0 and $0, \frac{1}{2}$ which also imply each other, so that in each of these cases there are only two types. In all there are twelve t types whose parameters are shown on the following table. (Only the v_i reduced values of the parameters u u, v_i , v_i are shown the others may readily be calculated by the equations above.

04,	lattic	77	parameters	0	0	0	0					
CAF	*	4	Ħ	0	0	sta-to	to to					
c _{4r}	*	ij	H (4) 2 3	0	100	0	0					•
C4.	•	1/		0	- to-to	- dow-jou	122					-
C4,	n ³	"	te!	1/2	0	0	0					
C4_			#	효	0	神の神	de de					
Cir	Ħ	Ą	W	ł	12/2	0	0					
C41-	•	•	•	1	104	to to	12/2					
C4"		<i>T</i> ,	n n	0	0	0	0	and	ł	o E	0 1 2	0 2
C **	, n	" #	. •	0	12/2	0	0	n n	12	1 0	0	0 2
C4,		٠	•	ł	0	20	Q E	11	3	0 3	0	10 to
Car	7	ft		1	1014	1 ST	0	**	\$	- torst	1012	0

47 D Derived from D by the addition of a centre of symmetry Y = -X+ua+yb+wc

As in the case of $C_{4,k}$ the only types of D from which types of D may be derived are are those for which u=0 or $\frac{1}{2}$ or wrere it $=0,\frac{1}{2}$; $\frac{1}{4},\frac{5}{4}$ at the same time namely D_4' , D_4' , D_4'' , D_4'' , D_4'' , D_4''

As in Q, u, v, w can take the values 0 and $\frac{\pi}{2}$ but since b and c are equivalent axes there are only four values 0 .0.0; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Thus each of $D_4^{'ij}$ give rise to four types. For $D_4^{''}$ uvw must be 0,0,0 or $\frac{1}{2}$,0,0 and for $D_4^{''}$ u,v,w must either be $0,\frac{1}{2}$,0 implying 0,0, $\frac{1}{2}$ or $\frac{1}{2},\frac{1}{2}$,0 implying $\frac{1}{2}$,0, $\frac{1}{2}$. $D_4^{''}$ and $D_4^{''}$ give rise to two types each. In all there are 20 types.

derived	from	D_4	parameters	0	0	0					
n	n	$\mathbf{D}_{4}^{\mathbf{z}}$	Ħ		11						
Ħ	w	D, s	11		ıı						
	17	D.	17		Ħ						
		D, '	n	Ì	0	0					
	*	D4	n		Ħ						
, #		D, 3	•		*						
		D,			n			٠.			
, w	n	D_4'	*	0	1	ł					
•	ň	D,	#		Ħ						
		D,	· •	•	n				r"	e -	to the Ni
ч 6 т	11	D,	**		н		10.5				
) w	*			Ì	1/2	1/2					
, ,		D,	L 11		n						
ስ // ਬ ਾਂ	Ħ				11	•					
	Ħ	D,	1 11 1		19						
// /7 w	**	D,	9 #	() (0					
	**			1	<u> </u>	0				:	
	*				0 (၁ နဲ့	and	0	ì	0	
#4 #4 #1			, No	-	} (o ½	. •)	ł	0	
	*** ** ** ** ** ** ** ** ** ** ** ** **	12 11 12 12 12 12 12 12 12 12 12 12 12 1		$\begin{array}{cccccccccccccccccccccccccccccccccccc$							

DA	derived	from	D_4	parameters	3 0	0 0)				
Dek	n	n	$\dot{\mathtt{D}}_{4}^{\mathbf{z}}$	Ħ		11					
D'	W ·	w	D. 5	n		ıı					
D,14		17	D.	π		н					
Den	•	*	D,	н	1	0 (3				
Dak	n .	*	D.	**		n					
D,	, #	Ħ	D,			*					
D.'3	11		D.4	•		Ħ					•
D ₄₄	, 4	n	D,	•	0	1	ì				
I	, , "	n	D,	.		Ħ					
\mathbf{D}_{4}^{n}	7.7. E 191		D.		•	п	,			٠.	*
D ,	7 6 · 11	11	D4	Ħ		11					
D ₄) w	*	D.	. *	. }	1 2	1/2				
D,			D,	11		n					
D,	n // Pr	. 1 1	D_4^4			71					
D,	15 st	w	D,	#		18					
ָם ב	// /7 w	**	D,	, n	(0 0	0				
	ρη /9 π 45	in				<u>}</u> 0	0				÷
	*^ /7 #	w				0 0	1	and	0	1	0
	<i>EU</i> 11		ת	,] 0	_	**	1	ł	0

.5 Rhombohedral Types

Five classes C_3 , C_{y_1} , D_{y_2} , C_{y_2} , D_{y_3} . Two lattices $T_A^{p_1}$, $T_{p_2}^{p_3}$

.51 C_3 the axis $Y = a^{\frac{1}{3}} X a^{\frac{1}{3}} + ua + vb + wc + x n$ to

The origin can always be chosen to make $\mathbf{v} = \mathbf{w} = \mathbf{t} = 0$ if can have the values 0, 1/3, 2/3 For Γ_h these are independent, the positions of the similar triad axes or screws can be found by 52 to be $\frac{m-n}{3} \cdot \frac{n-o}{3}, \frac{o-m}{3}$. For Γ_m the values 0, 1/3, 2/3 imply each other but these dissimilar axes pass through the same points. There are four types \mathbf{C}_j' lattice $\Gamma_h' \mathbf{u} = \mathbf{0}$; \mathbf{C}_3' lattice $\mathbf{C}_h' \mathbf{u} = \mathbf{0}$; $\mathbf{C}_3' \mathbf{$

$$C_3^4$$
 " $\Gamma_{n}' u = 0$ and $\frac{1}{3}$ and $\frac{2}{3}$

.52 C_{3i} Derived from 6 by the addition of an axis a centre of symmetry $Y = -X + u_A + v_b + w_C + t_A$

The origin can always be chosen to make u = 0.

As in the case of C_4 only the types C_3 and C_3 can give rise to a type of this class. By A we have: for both $\sum_{n=0}^{\infty} \sum_{n=0}^{\infty} x_n = \frac{n-n}{3}$; $x_n = \frac{n-n}{3}$; $x_n = \frac{n-n}{3}$; so that there are only the two types

 C_{jj}^{l} lattice T_{k}^{l} derived from C_{j}^{l} parameters 0 0 0 C_{jj}^{l} " T_{k}^{l} " " C_{j}^{l} " 0 0 0

53 D four axes Y = a Xa 4ua

 $\begin{array}{lll} Y = bXb^{-1} + ua + vb + wo + td \\ Y = CXc^{-1} + ua + vb + wo + td \\ Y = dXd^{-1} + ua + vb + wo + td \\ \end{array} \quad \begin{array}{lll} (c+d)X(c+d)^{-1} + c+c \\ (d+b)X(d+b)^{-1} + c+c \\ (b+c)X(b+c)^{-1} + c+c \\ \end{array}$

the two ways of writing the relations depend on the fact that both b,c,d and (c+d), (d+b), (b+c) can be taken as diad axes of the lattice Γ_k though only the first can be taken for Γ_{cl} .

Transforming 2 by 1 and equating to β , we obtain $u_z=u_z+2u_z$, $v_z=t_z$, $v_z=v_z$

this holds for both for both forms of the relations.

By 5.7% we have $v_1 = \frac{m-n}{3}$; $w_2 = \frac{n-o}{3}$; $t_3 = \frac{o-m}{3}$ but this is of the same form as we obtained for the axial parameters in C_3 so that only one type in each form corresponds to the three types C_3 , C_3 , C_3 , and only one of the first $\frac{f_{orig}}{g_{orig}}$ to C_3 , there are in all seven types.

D,	lattice	T ₄	parameters	0	0	0	-	0	Diad	axe	8	b,0,d	
D;	**	H	•				ŏ		Ħ	Ħ			(a+d), (d+b), (b+c
D,		n	·, •	13	g	0	0		11	11			•
ָם	5 H	# #	Ħ	Ĭ	Coup-day	0	0	0		n			# ,
D.	•	•	Ħ	<u>2</u> 3	0	0	0	0	*			#	
D	5 W	•	#		13213	0	0	0	w	0 0	0		•
D,	4	Į	,	0	0	0	0	000	and $\frac{1}{3}$	0 1313 3 1313	13730		13 0 13 13 13 13 13 13 13 13 13 13 13 13 13 13 13 1

.54 0 one axis and three planes

Y = -bXb' + ua + vb + wo + td or -(c+d)X(c+d)' + eto Y = -cXc' + ua + vb + wc + td -(d+b)X(d+b)'' + etoY = -dXd'' + ua + vb + wc + td -(b+c)X(b+c)'' + eto

Exactly as for D₃ we obtain u,=u,=u,v,=w,=t;w,=t,=v; t,=v,=w,=by 5.77u = 0 and by 51u,=0 or ½. Further as for D₃ there can only one of each sort.

set of independent values of v,w,t, Thus we have two types corresponding and two of the first sort.c. C₃
to each of C₃, C₄, C₅. In all six types.

.55 D, derived from D, by the addition of a centre of symmetry

Y = -X+ua+vb+wo+td

Exactly as in C_{j_1} we find that the only types of D_j that can give rise to types of D_{j_2} are D_{j_3}' , D_{j_3}'' , D_{j_3}'' , also that v_j , w_j , t_j always reduce to the same values 0,0,0. but in this case u_j can have the values 0 or $\frac{1}{2}$ so that to each of D_{j_3}' , D_{j_3}'' , corresponds two types, making six in all.

 D'_{3} corresponding to D'_{3} u = 0

.s Hazagonal Types

Seven classes C, C, C, C, D, D, D, C, D, One lattice

.61.0, the axis $Y = a^{\frac{1}{2}} I a^{\frac{1}{2}} + n a + v h + w a + t d$

The origin can always be chosen to make $\forall = w = t = 0$ u can have the values 1/6, 1/3, 1/2, 2/3, 5/6,

By 52 we can find the position of the hexad axes to be $\frac{21-m-n}{3}b$ +etc and as each axis is also a triad and diad axis there are such axes through the points $\frac{1-m}{3}b$ +etc and $\frac{21-m-n}{6}b$ + respectively.

There are six types C_4' , C_4' ,

There are six types C'_{a} , C'_{a} , C'_{a} , C'_{a} , C'_{a} , C'_{a} , with the six values respectively that are given above for u.

centre

.520 derived from C, by the addition of an exim of symmetry

Y = -X+us+vb+wc+td

As in C_{jj} we can see that the only types of C_{ij} from which types of C_{ij} can be derived are C_{ij} and C_{ij} , also that that u, v, w, t, always reduce to Thus there are only two types: C_{ij} derived from C_{ij} derived from C_{ij}

.53 G_{3k} The axis
Y= a Xa +ua +vb +wc +td

The origin can always be chosen so that u, v, w, t, 0, 0, 0, 0. There is only one type C_{12}'

.54 $D_{\chi l}$ The four axes, and the three planes

 $Y = -a^{\frac{1}{2}} \times a^{-\frac{1}{4}} + ua$ $Y = b \times b^{-\frac{1}{4}} + ua + yb + wc + td$ and $(c+d) \times (c+d)^{-\frac{1}{4}} + etc$ $Y = c \times c^{-\frac{1}{4}} + ua + yb + wc + td$ $Y = d \times d^{-\frac{1}{4}} + ua + yb + wc + td$ $Y = -(c+d) \times (c+d)^{\frac{1}{4}} + ua + yb + wc + td$ $Y = -(d+b) \times (d+b)^{-\frac{1}{4}} + ua + yb + wc + td$ $Y = -(b+c) \times (b+c)^{-\frac{1}{4}} + ua + yb + wc + td$

The relations between the parameters are similar to those in D, and C,

Here however u can be 0 org so that there two types of each sort.

D Seven axes
Y = a Xa +ua
Y = bXb +ua+vb+wc+th

The relations between are similar to those of D_3 . There are six types D_4' D_5' D_5' D_6' D_6' D_6' D_6'' D_6'' D

 $Y = a^{\frac{1}{2}}Xa^{-\frac{1}{2}} + ua$ Y = -bXb + ua + vb + wc + tA Y = -(c+d)X(c+d) + ua + vb + wc + tA

The relations between the parameters are similar to those of C_{j_p} u=0 or $\frac{1}{2}$, U $u=u_p$ u=0 or $\frac{1}{2}$ there are four types $C_{j_p}^{\prime}$ u=0; u=0; u=0; $u=\frac{1}{2}$; $C_{j_p}^{\prime}$ $u=\frac{1}{2}$; u=0; $C_{j_p}^{\prime}$ $u=\frac{1}{2}$; u=0; u=0;

$$D'_{6k}$$
 u = 0; u = 0. D^{2}_{6k} u = 0; u = $\frac{1}{2}$. D^{3}_{6k} u = $\frac{1}{2}$; u = 0 . D^{4}_{6k} u = $\frac{1}{2}$; u = $\frac{1}{2}$

.7 Regular Types.

Five classes T , T, T, O , Q . Three lattices T, T, C

.71 T seven axes

Y = axa + ua + vb + wo Y = bxb + ua + vb + wo Y = cxc + ua + vb + wo

Y = $(a+b+c)^{2}X(a+b+c)^{-\frac{1}{2}}+ua+vb+wc$ Y = $(a-b-c)X(a+b+c)^{-\frac{1}{2}}+ua+vb+wc$ Y = $(a+b-c)X(a+b-c)^{-\frac{1}{2}}+ua+vb+wc$ Y = $(a-b+c)X(a-b+c)^{-\frac{1}{2}}+ua+vb+wc$

As I. I may all be considered as special forms of I we must accordingly have rotation axes in the direction of each of the triad axes.

the origin may accordingly be chosen to lie on the rotation axis triad a4b+c so that u, v, w, O also the parameters of the other sectation axis can always be made to refer to rotation axes if u-v-w; -u-v-w; -u-v-w, respectively are made = 0.

Trans-forming 1 by 4 and equating to 2 , and similarly for 2 and 3 we have the conditions $u_i = v_i = w_i$; $u_i = v_j = w_i$; $u_i = v_j = w_i$.

Now, T may also be regarded as a special form of Q then the only types of Q to which types of T may correspond are those which satisfy the above conditions namely Q^1, Q^1, Q^2, Q^3 so that there five types of T.

Transforming 4 by 1 and equating to 5 we have u₅·u,+w₁; v₅·v,+u₁; w₅·w,-v₇·v,

4 2 " 2 6 " u₅·u,-w₁; v₇·v,+u₁; w₇·w,-v₈·v,

4 3 " " 7 " u₁·u,+w₃; v₇·v,-v,+u₂; w₇·v,-v,+v₈·v,

T' lattice \(\times \) corresponding to \(\text{Q}' \) parameters \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 0 \(0 \) 1 \(\frac{1}{2} \) \(\

T	lattice Coor	rresponding to Q [†] parameters	0 0 0 0 0 0 0 0 0	110	65 - to to 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
T	, Ľ,	"	000		# # 0 # # # # 0 #
T'	* Ç*	e e e e e e e e e e e e e e e e e e e	0 0 0 0 0 0 0 0 0 0 0 0 0		•
			0 0 0 0 1 0 1 0 1 0 1 0 1 0 1 0 0 1 0 1	0-10-10-10-10-10-10-10-10-10-10-10-10-10	A CO

72 I Derived from I by the addition of a centre of symmetry

Y= +X +un+yb+wg

As in the case of Q_i the only possible values for u_i, v_i, w_i are 0 or $\frac{1}{2}$ but by the trigonal symmetry $u_i = v_i = w_i$ so that these reduce to two 0 0 0 and $\frac{1}{2}$ $\frac{1}{2}$ but just as in Q^i we have for T^i 0 0 0 and $\frac{1}{2}$ $\frac{1}{2}$ are indistinguishable and in T^i and T^i they imply each other so that only T^i and T^i give rise to two types of T_k thus making 7 inhall. T_k^i lattice Γ derived from T^i parameters 0 0 0

$$T_{h}^{2}$$
 " Γ_{r}^{2} " " T_{r}^{2} " " T_{h}^{2} " T_{h}^{2} " T_{h}^{2} " T_{r}^{2} " " T_{r}^{2} " " T_{r}^{2} " T_{h}^{2} " T_{r}^{2} " " T_{r}^{2} " " T_{r}^{2} " $T_$

.73 T Derived from T by the addition of the six planes

```
Y= -(b+c)X(b+c) +ua+yb+wo

Y= -(b-c)X(b-c) +ua+yb+wo

Y= -(c+a)X(c+a) +ua+yb+wo

Y= -(c-a)X(c-a) +ua+yb+wo

Y= -(a+b)X(a+b) +ua+yb+wo

Y= -(a+b)X(a-b) +ua+yb+wo
```

This class may be considered as a special case of both D_{1d} and C_{3v} .

From the first we see that as there is no type of D_{2d} corresponding to Q^* there can be no type of T_{2d} corresponding to T^* . From the second we see that as in C_{3v} , C_{3v} or C_{2d} so C_{2d} for C_{2d} and C_{3v} or C_{2d} is the only type of C_{2d} corresponding to C_{2d} and C_{3v} is the only type of C_{2d} corresponding to C_{2d} and C_{3v} is the only type of C_{2d} corresponding to C_{2d} and C_{3v} is the only one type corresponding to C_{3v} in C_{3v} is the only one type corresponding to C_{3v} in C_{3v} in C_{3v} is the only one type corresponding to C_{3v} in C_{3v}

.74 O Derived from T by the addition of the six axes

$$Y = (b+c)X(b+c) + ua+vb+wc$$

$$Y = (b+c)X(b+c) + ua+vb+wc$$

There in all then eight types. As the class 0 has tetrad axes in the place of the diad axes of T the parameters u, v, w are given as well as u, v, w

0'	lattic	e Çeori	responding	to T'D, pa	arameters	000		
01		r		T' D	*	1 0 0 0 1 0 0 0 1 2 0 0 2 0 0		
0,	£	Ľ,	• • • • • • • • • • • • • • • • • • •	T' D'		0 0 0 0 0 0 0 0 0 0 0 0	-to-to-to-to	
o*	•	た	* · · · · · · · · · · · · · · · · · · ·	T' D'	• · · · · · · · · · · · · · · · · · · ·	\$ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	-ta-tarje ta -tarje ta-ta	
0,	•	Γ,"	•	T ^S D,	A	0 0 0 0 0 0 0 0 0	-ta-ta-ta-ta-ta	
04	•	Ţ	11	T [*] D [*]		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		75
oʻ	•	<i>P</i> ₊	•	T ⁴ D ⁴ ,		0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		स्रो
O ^s	n	Ţ,*	•	T" D"	•	10000		

.750 Derived from 0 by the addition of a centre of symmetry Y = -X +ua+vb+wc

As in the case of D_{44} we can only derive types of this class from classes corresponding to $D_4'D_4''D_4''D_4''D_4''D_4''$ namely O'O'O'O'O',

For Γ_r we have u = v = w = 0 or $\frac{1}{2}$ For $\Gamma_r u = 0$ $\frac{1}{4}$ $\frac{1}{2}$ but for 0^3 , 0 implies $\frac{1}{2}$ and $\frac{1}{4}$, $\frac{3}{4}$ while for 0^4 u cannot have the values 0 or $\frac{1}{2}$ so that in each case only two types are derivable. For $\Gamma_r''u = 0$ implies $u = \frac{1}{2}$ so that only one t type corresponds to each of 0^4 and 0^6 . In all there are ten types

tуļ	be corres	ponde	,	980H 01	o and	•
0'	derived	from	0' p	arameter	8 0 0	0
0*	n	n	o'	**	1 1	12
0,	•	n	0		0 0	0
of	**	*	o*	**	1 1	1/2
05	w :	*	03		0 0	0
0	n	*	03	11	1 1	ł
o'	W	**	04	: n	11	1
08			o		3 3	\$
01	*	**	05	70	0 0	0
\ 10			~ \$			^

COMPONENT SETS

E

•11

.1 Equivalent points

We have already deduced all the symmetry relations of the 230 types of point systems. By means of these we can in any system write down the vectors of all the points equivalent to a given point.

If the reduced relations of any system be given by $Y^{\pm}(-1)^{i}A^{\frac{f_{i}}{f_{i}}}X\tilde{A}^{\frac{f_{i}}{f_{i}}}+B_{i}$ $Y^{\pm}(-1)^{i}A^{\frac{f_{i}}{f_{i}}}X\tilde{A}^{\frac{f_{i}}{f_{i}}}+B_{i}$

where h has all the values 1,2,....k for each of the n values of k_{\perp}

The number of such equivalent points in a component set can only depend on the retational part of the relation, so that in what follows we will deal only with this part.

Now since $Y=(-1)^{k_1} A^{\frac{k_2}{k_1}A^{\frac{k_2}{k_1}}}$ reduces to Y=X (except in the cases where V=1 and $k_1=1$ or 3 when it reduces to V=X) and there are n relations of this type, there are in general $\sum_{i=1}^{k_1} k_i - n$ points equivalent to any point and in all

\$k_r-n+l points in the set.

If there is a rotation of the type Ym-X there are

2k,-n+2

and if there m of the type Ym -A XA there are

 $\sum k_r - n + 5m + 1$ points in the set

•12 Alternatively we may start with the independent reduced relations $/ Y = (-1)^{n} \hat{A}_{XA}^{\frac{n}{n}}$

all points equivalent to X are given by:

$$Y = (-1)^{\sqrt{2} \frac{2}{\Lambda}} A^{\frac{2}{\Lambda}} A^{\frac{2}{\Lambda}} \dots A^{\frac{2}{\Lambda}} X A^{\frac{2}{\Lambda}} \dots A^{\frac{2}{\Lambda}} A^{\frac{2}{\Lambda}} A^{\frac{2}{\Lambda}} A^{\frac{2}{\Lambda}}$$

where h has all the values $0,1,2,\ldots(k-1)$ The number of equivalent points is in general

$$k_1 k_2 \cdot \cdot \cdot \cdot k_n$$

As before the existance of a relation $Y_{\Xi}-X$ doubles the number of equivalent points; but we need not consider the effect of $Y_{\Xi}-A^{\frac{1}{2}}XA$ since it can always be derived from $Y_{\Xi}-X$ and $Y_{\Xi}A^{\frac{1}{2}}XA$. Sometimes the first, sometimes the second method is the most equivalent for deriving the equivalent points.

•18 In the following table there is given for each class of rotation the most natural way of doing this.

Note Abbreviations used

At denotes the relation $Y=\Lambda^{\frac{1}{k}}XA^{-\frac{1}{k}}$ -At " " Y=- $\Lambda^{\frac{1}{k}}XA^{-\frac{1}{k}}$ 1 " Y=- $\Lambda^{\frac{1}{k}}XA^{-\frac{1}{k}}$ + " " Y=- $\Lambda^{\frac{1}{k}}XA^{-\frac{1}{k}}$

 $(A_1^{\frac{1}{1}}, A_L^{\frac{1}{1}}, A_L^{\frac{1}{1}}, A_L^{\frac{1}{1}}, A_L^{\frac{1}{1}})$ signifies that every pair relation in the first bracket is to be combined in turn with each one in the second, and similarly for products with more than two brackets

Symbol of class	Group of rotations		es of Lent_points
c,	1	•	1
Cį	±1		2
C,	1,-A		2
C,	1, A		2
Czk	±(1,A)		4
C _{2p} .	1, A,-B,-C		4
Q	1, A, B, C	٠	4
Q,	±(1, A, B, C)	*	
c,	1, A, A, A, A		4
C,	1, A, A, A, A		4
C4A	±(1, A, A, A, A,)		8
Dzd	$(1,A,A,A^{\frac{1}{2}})(1,B)$		8
C	(1, A, A, A, A,) (1,-B)		8
D ₄	$(1, A^{i}, A, A^{i})(1, B)$		8
D	$\pm(1,A^{\frac{1}{2}},A,A^{\frac{1}{2}})(1,B)$		16
C ₃	1, A, A		3
Cyt	±(1,*A, A,*)		6
Csp	(1,A,A,)(1,B)		6
$\mathbf{D_{3}}$	(1,A,A,)(1,B)	•	6
D _M	$\pm (1, A, A^{\frac{5}{7}})(1, B)$		12

Symbo of cla		ons Number of equivalent points
C _{J4}	(1,A)(1,A,A,A,	.
DSA	±(1,-A)(1,A,A)	12
C.	1, A, A, A, A, A	6
C	(1, A,	;B) 12
D4	(1, A, A, A, A, A, A ^f) (1	,B) 12
Dea	±(1, A,	,B) 24
T	(1, A, B, C)(1, T, T	· [‡]) 12
T	±(1, A, B, C)(1, T, T	(4)
T	(1, A, B, C)(1, T, T)	1,R) 24
0	(1,A,B,C)(1,T,T,T)(1,R) 24
O _Á	±(1, A, B, C,)(1, T, T, T,)(1,R) 48

•2 Coordinates

In general we refer the points of a system to three reference vectors, and the position of any point is given by its coordinates λ, μ, ν with respect to these vectors. (In the rhombohedral and hexagonal systems four reference vectors are employed.)

•21 If we write $X = \lambda a + \mu b + \nu c$; $Y = \lambda a + \mu b + \nu c$ in the relation $Y = (-1)^{\frac{1}{A}} X A^{\frac{1}{A}}$ it becomes

$$\lambda \hat{a} + \mu \hat{b} + \nu \hat{c} = (-1)^{\lambda} \hat{a}^{\dagger} (\lambda \hat{a} + \mu \hat{b} + \nu \hat{c}) \hat{a}$$

$$= (-1)^{\lambda} \hat{a} \hat{a}^{\dagger} \hat{a}^{\dagger} (-1)^{\lambda} \hat{a} \hat{a}^{\dagger} \hat{a}^{\dagger} \cdot (-1)^{\lambda} \hat{a} \hat{c} \hat{a}^{\dagger}$$

$$= (-1)^{\lambda} \hat{a} \hat{a}^{\lambda} \hat{a}^{\dagger} = (-1)^{\lambda} \hat{a} \hat{a}^{\dagger} \hat{a}^{\dagger} \cdot (-1)^{\lambda} \hat{a} \hat{c} \hat{a}^{\dagger} \hat{a}^{\dagger} \cdot (-1)^{\lambda} \hat{a} \hat{c} \hat{a}^{\dagger} \hat{c}$$

Now $(-1)^{\frac{1}{2}}$ = 1a+mb+nc $(-1)^{\frac{1}{2}}$ = 1a+mb+nc $(-1)^{\frac{1}{2}}$ = 1a+mb+nc $(-1)^{\frac{1}{2}}$ = 1a+mb+nc

where 1, 1, 1, etc are integers

Equating coefficients of a,b,c we have

The relations between the coordinates of two points connected by a rotation can be expressed in the form of a matrix

Since the inverse of a rotation is a rotation, this matrix must have the property $\begin{vmatrix} 1 & 1 \\ m & m \\ n & n \end{vmatrix} = \pm 1$

In the following table are given the matrices corresponding to a number of rotations, together with the values of $\lambda \mu^{r}$ in terms of $\lambda \mu v$.

23	Rotation	Matrix	The state of the s	Coordinates
	1	1 0 0 011 0 0 0 1		λ, μ. ν.
	-1	-1 0 0 0-1-0 0 0-1		-λμ . - ν.
	8	1 0 0 0-1 0 0 0-1		: · · λ , -μ, - ν ,
	-8	-1 0 0 0 1 0 0 0 1		-λ, μ, y
	b	-1 0 0 0 1 0 0 0-1		-λ.+μV
	-b	1 0 0 0-1 0 0 0 1		λ,-μ,ν
	G	-1 0 0 0-1 0 0 0 1		- <i>λp</i> , v
	-0 4	1 0 0 0 1 0 0 0-1		λ. μν
	R = [b+c]	-1 0 0 0 0 1 0 1 0		-λ, ν, μ
	-R = [b+c]	1 0 0 0 0-1 0-1 0		λ,-γ,-μ
	at	1 0 0 0 0-1 0 1 0		λ,-ν, μ
	-a t	 -1 0 0 0 0 1 0-1 0	en de la companya de La companya de la co	-l, v,- µ

in the most general point system we add to the coordinates of the equivalent points derived by rotations the corresponding parameters of the general relation

Here
$$\lambda' = 1, \lambda + 1, \mu + 1, y + u$$

$$\mu' = m_i \lambda + m_i \mu + m_i v + w$$

$$v' = n_i \lambda + n_i \mu + n_i v + w$$

and similarly for every relation of the system.

The parameters can be taken from the various tables of Ch.VI
the rotations are given in table 7.13 and their matrices in
table 7.22.

For example in the system Q, we have for equivalent points $\lambda,\mu,\nu \ ; \lambda,-\dot{\mu}+\frac{1}{2};-\dot{\nu}; \ -\dot{\lambda}\,\dot{\mu}+\frac{1}{2};-\dot{\nu}+\frac{1}{2}; \ -\dot{\lambda},-\mu,\nu+\frac{1}{2}$ These will appear in a more symmetrical form **x** if we put $\mu+\frac{1}{2} \text{ for } \mu,\ \nu+\frac{1}{2} \text{ for } \nu.$

$$\lambda$$
, $\mu + \frac{1}{4}$ $V + \frac{1}{4}$
 λ , $-\mu + \frac{1}{4}$ $-v - \frac{1}{4}$
 $-\lambda$, $\mu - \frac{1}{4}$ $-v + \frac{1}{4}$ Here $-\frac{1}{4}$ has been written for $-\lambda$, $-\mu - \frac{1}{4}$ $v + \frac{1}{4}$

·3 Unit cells

As has been already shown (1.8) we can always choose certain limits for the coordinates of the points in a component set. Such limits mark off a portion of space inside of which all the points of a component set may lie, such a portion is called a unit cell. There is one unit cell corresponding to every point in the skeletal lattice.

Two alternative limits were suggested $(AV \le \lambda, \mu, v \le 1/2) \le 1/2 \lambda, \mu, v \le 1/2$ (B) will be used in what follows. The unit cell has thus the shape of a parallopiped whose centre is at the origin; a point of the set may lie anywhere inside this cell, on three of ats faces, three of its edges and one of its angular points. This arrangement is unsymmetrical but if we make the limits $-\frac{1}{2} \le \lambda, \mu, v, \le \frac{1}{2}$ so that points may lie on all the faces edges and corners, such points must count as $\frac{1}{2}, \frac{1}{4}$ and $\frac{1}{8}$ of a point respectively whach is liable to cause confusion.

The above limits for the unit cell are only usefulk for the lattices $\Gamma_{r}, \Gamma_{r}, \Gamma_{r}, \Gamma_{r}$. If we write the formula of any other lattice in terms of its primitive vectors and introduce these limits we obtain unit cells which do not possess the symmetry of the system.

The limits for cells satisfying this condition for each of the 14 lattices, are given with their descriptions, in the following table.

Lattice	Limits f		Description of cell
T_{t_T}	-2< y < 2 -2< y < 2 -2< y < 2		Parallelopipedon
T _m	st		Oblique rectangular prism
r,	Fig. 1	N N 3	Rectangular rhombic prism
T _e .	- " H		Tetragonal prism
T_{r}^{r} .	~ - 18		Cube
L .	-= < \ + + + = = = = = = = = = = = = = = = =		Clinodomal prism and pinacoid (Oblique prism on rhombic base)
" ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' '	-\frac{1}{2} < \lambda < \frac{1}{2} -\frac{1}{2} < \lambda + \frac{1}{2} -\frac{1}{2} < \lambda - \frac{1}{2}		Primary rhombic prism (Rectangular prism on rhombic base)
7 *	++++++++++++++++++++++++++++++++++++++		Rhombic, macro- and brachy- domal prisms; ((Elongated dodecahedron)
L **			Rhombic dodecanedron second order to Rhombic byryramid and pinacoids (Elongated truncated octahedron)
<u>'</u> '			Tetragonalbipyramid second order prism and pinacoids. Octahedron and cube; (truncated
Ţ	-½ -1<2µ-4-61 -1<-µ-4-61 -1<-µ-4-61	· · · · · · · · · · · · · · · · · · ·	octahedron) Hegagonal prism and pinacoids
T	-{<21-44 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{<57-6+4 -{ 57-6+4 -{ 57-6	1	RHOLIBOHEDRON

Submultiple sets

If X is such that the relation Y= \$1)A A B reduces
to Y=X then the relation A B does not increase the number
of points equivalent to X, derived from the other independent
relations. The total number of points equivalent to X will
accordingly be 1/k, the number for the most general value of X
Such a set of equivalent points is called a submultiple or subset. If in addition another independent relation of the set
reduces to Y=X we have a subset, 1/kk, the full set, and we may
ultimately arrive at a sub set containing only one point.

•41 The relation $Y = (1)^{A} XA^{\frac{2}{3}} + hA/k + B$ reduces to Y = X in the following cases. (a) If y = 2 and h = 0 X = pA + C where $A^{\frac{2}{3}}CA^{\frac{2}{3}} - C + B = 0$ if B = 0. C = 0. (d) If y = 1 and $k \neq 2$ X = hA/2k + C " $A^{\frac{2}{3}}CA^{\frac{2}{3}} + C - B = 0$

Expressing this in words; A sub set can be formed when, and only when, its points lie on (a) axes of rotation. (See 5.2 at seq set example: The 48 pointer full set of 0_{λ} reduces to a 24 pointer sub set when $\lambda = \mu = V$; to a 6 pointer when $\lambda = \nu = 0$ and to a 1 pointer when $\lambda = \mu = V = 0$.

consider the case of a multiple point system containing axes of screw symmetry or glide planes which have no rotation axes or reflection planes parallel to them. If a point lie on such an axis or plane the number of points will only be reduced by a rotation included in the screw axis if any such exist.

In no case can the number of points in the sub set reduce to one. All non equivalent points in a multiple system connot lie on the same screw axes or glide plane. In this case relation an equation of the type YEAXA + hA/k reduces to YEX + hA/k or in the case of a glide plane YE-AXA + B/2to YEX + B/2 which would imply that A/k and B/2 were vectors of the skeletal lattice.

- All the points of a multiple system however can only form subsets of one in holohedral classes. Similar conditions hold for all other sub sets. If we consider simple systems only we have for each class a sub set that exhibits the symmetry of the class with the least number of points.
 - In the following table is given a list of sub sets for every class with sub sets characteristic of it. In these classes the last sub set, and in all other classes the full set, is the least sub set. The values of A, M, V for each sub set are also given.

Class	Sub set	Number in sub set	Class	Sub set	Number in sub set
cį	λ=μ=V=0	1	D saf	V= 6	. 6
•		•	H	v=-e	6
Csh	λ = 0	2	10	X= = = = 0 = 0	1
CA	µ = v = 0	12		•	
11	λ= μ = V = O	1	C _{3.6}	λ=0	3
			D,X	V=6	6
5	λ = 0	4	CEA	1=6	6
· If	µ= V=0	. 2	Du	X = 0	12
- - 11 -	\ = \ = \ \ = 0	1 .	- εξ	v = 6	12
				λ=0 V=P	6
Du		4		µ=v=P	2
CAA	λ=0	4 Salago en Bran	er De la N	· λ=μ=ν=θ=ι	
D_{AB}	1=0	8	19	· / = / = (= (1
11	µ=0 or µ=V	8			
11	1=0, 4=0 or #	•/ 4			
, "	µ=V=0	2			
178	λ= μ = V = 0	1			
	•			San Harry	
T	λ=0	12			
T	μ=V	12			
o _k	•	24			
	A = 0	24	•		
, 11	μ-ν, λ=0	12			
	1= N= V	8			
n	µ= v=0	6			
. 11	λ= μ = V = (

•45 Available positions

The points of a sub set must lie either on rotation axes unit cell in any or reflection planes. There are thus in every point system a fint finite number of planes, lines and points in which the points of sub sets must lie. All the points of the component included set may be located there only in those classes in the foregoing table. The case of one point sub sets is peculiar; in that only a limited number of such sub sets can co-exist in any system. Only a certain number of systems can reduce to one point sub sets, other systems can only reduce to two pointers and so forth.

(At this point it was hoped to be able to introduce a table showing every sub set possible in each of the 230 systems for the together with the available positions of such sub sets.)

of the paper. 2003.

CHAPTER VIII

PLANES_

.1 The equation to a plane

If the variable vector X be expressed in terms of the vectors a,b,c then the so that X=pa+qb+rc; then the existance of an equation of the type

$$fp+gq+hr+J=0$$

between the variable scalars p,q,r and the constant scalars f,g,h,j indicates that the extremity of X must always lie on a plane determined by f,g,h,j.

If X is a vector of a point system the values of p.q.r are restricted. All permissible values of p,q,r which satisfy the equation fp+gq+hr+j=0 indicate points of the system lying in the plane f,g,h,j. Should any such points exist, the number of them is given by the number of permissible solutions of the above equation.

2 The law of rational indices

p,q,r can always be put in the form $/1+\lambda_1$, $m+\mu_1$, $n+V_2$; where 1, m, n can take all integral values $-\frac{1}{2} \cdot \lambda_1 \cdot \frac{1}{2} \cdot \lambda_1$ and z is finite.

If any point corresponding to $\lambda_1 \mu_1 V_2$ be on the plane we have

$$f(1+\lambda) \cdot g(m+\mu) + h(ii+V) + j = 0$$

or fl-gm-hn+j = 0 where j = fA+gA, +hV,+j
this is an equation which only admits of integral solutions,
there will be a doubly infinite set of these if and only if
f,g,h,j are all rational multiples of the same irrational number.

By multiplying by a suitable factor f,g,h may be reduced to integers with no common factor; in this form f,g,h are called the indices of the plane. In the subsequent work we are only concerned with sugh planes; the term plane will refer exclusively to planes containing a doubly infinite system of points, corresponding to a gaven point of the three dimensional point system. As all, points form lattices, we will in the following sections consider lattices only.

•3 Formula of a plane net

The points of the lattice /la+mb+nc which lie in the plane fl+gm+hn+j=0 form a two dimensional net. We can obtain the formula of the net by eliminating l,m,or n from the formula of the lattice by means of the equation of the plane. The following proceedure is however more symmetrical.

Let $u_1, v_1, w_1; u_2, v_2, w_2$ be two points on the plane fl+gm+hn=0 and u_3, v_3, w_3 be a point on the plane fl+gm+hn+j=0 the general solution to the equation of the plane may now be written

$$1 = su_{i} + tu_{i} + u_{j}$$

$$m = su_{i} + tu_{i} + v_{j}$$

 $n=sw_1+tw_2+w_3$ Introducing these values into the formula of the lattice we obtain the formula of the net

as
$$/(su_1 + tu_2 + u_3)a + (sv_1 + tv_2 + v_3)b + (sw_1 + tw_1 + w_3)c$$

or $/s(u_1a + v_1b + w_1c) + t(u_2a + v_2b + w_2c) + (u_3a + v_3b + w_3c)$
writing $(u_1a + v_1b + w_1c) = e_1$; $u_2a + v_2b + w_2c = e_2$; $u_3a + v_3b + w_3c = e_3$
the formula becomes $/se_1 + te_2 + e_3$

If the plane passes through the origin e = 0 and the formula of the net reduces to /se +te,

e, and e_i will be primitive vectors of the net if e_i e_i e_j are for the system, lattice. That is if

If we substitute for the first column, that formed by multiplying the columns by f.g.h respectively and adding.

we have
$$\begin{vmatrix} 0 & v_1 & w_1 \\ 0 & v_2 & w_3 \\ -j & v_3 & w_3 \end{vmatrix} = \pm \mathbf{f}$$
Expanding
$$\begin{aligned} v_1 & w_2 - v_2 & w_1 = \pm \mathbf{f}/j \\ w_1 & u_2 - w_2 & u_3 = \pm \mathbf{g}/j \\ u_1 & v_2 - u_2 & v_3 = \pm \mathbf{h}/j \end{aligned}$$

Since /u, are all integers and f,g,h have no common factor j=1, but the condition that e, and e, should be primitive is independent of the value of e, and consequently of j: this condition as therefore v, w, -v, w, -tf

$$W_1 U_1 - W_2 U_1 = \pm g$$

$$U_1 V_2 - U_1 V_2 = \pm h$$

•4 Parallel planes

Planes with the same values of f,g,h but with different values of j are parallel. If the indices are expressed in terms of primitive vectors j must be an integer and as no plane can lie between the parallel planes f,g,h,j and f,g,h,(j+1), these are called succesive planes.

•5 Distance between planes

The perpendicular distance from the origin to the plane fl+gm+hn-1=0

may be expressed as the quotient Volume of //pipedon e, e, e, Area of //gm e, e,

Now /u, can always be chosen so that $(u, v, w_3) \implies 1$ also (v, w, -v, w) = f etc. We have therefore

Perpendicular distance
$$n = \frac{Sabc}{T(fVbc+gVca+hVab)}$$

This expression may of course be derived directly from the equation of the plane and is true for all real values of f,g,h,j In its most general form it is

$$D_{i} = \frac{1Sabc}{T(fVbc+gVca+hVab)}$$

This equation expression though simple is not convenient for numerical calculation as it involves sums and products of vectors. It can easily be transformed however into one that is.

•51 We make use of the formula -(Sabc) = S.VbcVcaVab (see Joly "Manual of Quaternions" Art. 25, Ex. 4)

-(Sabo) = S. Vbc Vca Vab

= S(bc-Sbc)(ca-Sca)(ab-Sab)

=S becaab-{Sbc.caab+{SbcSca.ab-SbcScaSab

=abc+fa(sbc)-3sbcScasab+SbcScaSab

= abc+a(3bc)+b(Sca)+d(Sab)-2SbcScaSab

Also f(fVbc+gVca+hVab) = f(Vbc)-25ghS.VcaVab
= f(Vbc)-25gh(a5bc-ScaSab)

We have therefore

$$\mathcal{D}_{i}^{2} = \frac{\text{ribc-} 2\text{si}(\text{Sbc}) + 2\text{JbcScaSab}}{2\text{EVbc}}$$

How if we put a for the scalar Ta, cos A for 3.UbUc; sinA for TV.UbUc and similarly for b and c; B and C the expression takes a form involving scalars only

$$\mathcal{D}^{2} = \frac{\text{abc}(1-\cos^{2}A-\cos^{2}B-\cos^{2}C+2\cos A\cos B\cos C)}{\text{form A -2coph(cos A + \cos B\cos C)}}$$

Finally we obtain the familiar formula

This formula loses much of its complexity when applied to symmetrical lattices. It is given for each of the 14 lattices in the table on p 94.

So far we have only considered lattices whose formula is written /la+mb+nc. It is not always convenient to use such a formula. For all lattices except , Γ_{k} , Γ_{rk} , , the formula may be written /(41+6m+yN)/2+(41+6L+yn)b/2+(41+6m+yN)c/2 (for Γ_{k} , Γ_{k} , Γ_{k} , Γ_{r} , $\Gamma_{$

f(x|1+0m+yn)/2+g(x|1+0m+yn)/2+h(x|1+0m+yn)/2+j=0

f.g.h may be such that exch of the first three terms is an integer for all values of 1,m,n.

In this case j is an integer and succesive planes are at the same distance as in the corresponding lattice /la+mb+nc

the tann of

If the first three terms do not reduce to integers j must be

of the form k/2 when k is an integer and successive planes are

half as far apart as in the corresponding lattice.

If d_{jk} stands for the distance between succesive planes parallel

to fp+gq+hr=0 in any lattice, and D_{jk} for the distance in a

corresponding lattice of formula /la+mb+nc, then d_{jk} f_{jk}D_{fk}

where S_{jk} depends both on the lattice and on f,g,h and is always

1, 2 or in the case of f_k1/3. The value of S_k for all lattices

and values of f,g,h is given in the table on p 94.

•53 The case of $\int_{\mathcal{A}}$ and $\int_{\mathcal{A}}$ must be dealt with separately; in this case four reference vectors are used and the equation of the plane becomes $f_{p+gq+hr+is+j}=0$ where $g_{p,j}$ are connected by the relation $g_{p,j}$ in this

fp+gq+hr+j = 0 is the equation of the same plane referred to the three vectors a, b, c Now applying the formula for D we have $D = \sqrt{\frac{3}{4}(f/a)^2 (g^2 + h^2 + gh)/b^2} \quad \text{since } \cos A = -\frac{1}{2} \cos B = \cos C = 0$ $= 1/\sqrt{f/a^2 + \frac{4}{3}(g^2 + h^2 + (h+1)(g+1))/b^2} \quad \text{since } g+h+1 = 0$ $= 1/\sqrt{f/a^2 + \frac{4}{3}(g^2 + h^2 + 1^2 + h^2 + gh)/b^2} \quad \text{since } g+h+1 + h^2 + g+g+1$ $= \frac{1}{2}(g+h+1) + \frac{1}{2}(g^2 + h^2 + 1^2 + g^2 + g^2 + h^2 + 1^2 + g^2 + g^2$

The formula of I_h^r is

/1a+(2m-n-o)b/3+(-m+2n-o)c/3+(-m-n+2o)d/3

= k(e+h+1)

g(2m-n-o)/3+h(-m+2n-o)/3+i(-m-n+2o)/3 is an integer when m(2g-h-i)/3+n(-g+2h-i)/2+o(-g-h+2i)/3 is an integer that is 2g-h-j is divisible by 3. In this case 1 and in all ather cases 1/3 But 2g-h-i=3g and is therefore always divisible by β so that for this lattice $\delta=1$

The formula of Lis

/(1+m+n)a/3+(m-n)b/3+(n-1)c/3+(1-m)d/3

by similar reasoning we can show that if f-h+i is a multiple of 3 $\delta = 1$ and if not $\delta = 1/3$

Forms

We now return to the most general point system.

The plane parallel to fl+gm+hn=0 through the point $\lambda \not \sim V$ is fp+gq+hr+j=0 where j (no longer necessarily an integer) is given by $f\lambda+g\mu+hV+j=0$

where $\mathbf{l}', \mathbf{l}'_{i}$ etc are the minors of $\mathbf{l}, \mathbf{l}_{i}$ l, in th matrix $(\mathbf{l}_{i} m_{i} n_{j})$ of the rotation. In other words $(\mathbf{l}'_{i} m'_{i} n'_{i})$ is the matrix of the inverse rotation $Y = (\mathbf{l})^{\lambda} \mathbf{l}^{\lambda} \mathbf{l}^{\lambda}$. For substituting for/ λ' and f' in terms of h and h we have

$$\frac{1}{2} \frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{1} + \frac{1}{2} \frac{1}{1} \frac{1}{1} \frac{1}{1} + \frac{1}{2} \frac{1}{1} \frac{1}{1} \frac{1}{1} = 0$$

$$- \frac{1}{2} \frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{1} + \frac{1}{2} \frac{1}{1} \frac{1}{1}$$

The planes fgh, and f,g,h, j are said to be equivalent planes.

If the symmetry relation is of the type Y=(1)A XA +ua+vb+wc the plane equivalent to f,g,h,j is f,g,h,j, where f,g,h are as K before but j=fu+gv+hw+j

- constitute a form. A form has the same number of planes as the number in the full set of equivalent points of the system.

 For certain values of f.g.h however k planes of the form coincide, and a sub form results each of whose planes contains k equivalent points, unless these points themselves form a sub set. (planes Such planes must be perpendicular to rotation axes or reflection. The same considerations that applied to the limitation of points in component sets apply to forms also, except that in this case j alone has to be limited.
 - If the system contains no screw axes or glide planes to which there are no parallel rotation axes or reflection planes, the form is called an infinite form; otherwise it is a finite form.

 Infinite forms may in certain cases contain up to 6 parallel the case of a planes. Consider for example the fiplane i,0%0,0 perpendicular to the screw axis $Y = a^{\frac{1}{2}} x a^{-\frac{1}{2}} + a/k$. The planes contained in the form are 1,0,0,0;1,0,0,1/k;1,0,0,2/k;1,0,0,(k-1)/k all of which are parallel.

By the symmetry of the system all the planes of a form must be congruent.

•7 Densities of systems and planes

•71 The point density of a system is defined as the number of points per unit volume of the system; aor alternately as

Number of points in unit cell Volume of unit cell

The number of points in a unit cell is simply the number N of points in a component set; the volume of a unit cell is Sabo when a,b,c are primitive vectors, in general however it is Δ Sabo where $\Delta = \begin{bmatrix} 1 & 1 & 1 \\ m & m & m \end{bmatrix}$ and $\Delta = \begin{bmatrix} 1 & 1 & 1 \\ m & m & m \end{bmatrix}$ and $\Delta = \begin{bmatrix} 1 & 1 & 1 \\ m & m & m \end{bmatrix}$ in terms of primitive vectors.

The values of Δ for each of the 14 lattices is given in the table on p 94. We have there fore as an expression for the point density $\frac{\Delta N}{Sabo}$

The point density of a plane may be defined as

Number of points in the plane per unit cell Area of unit cell

If n is the number of points of a component set that lie in the plane and δ and Δ have the same meaning as in the preceding sections; Point density $\frac{n}{\delta}$

$$= \frac{\delta \Delta n}{T(fVbc+gVca+hVab)}$$

•73 Weighted densities

In a multiple system we may attribute to each point a weight factor m,; m, being the same for all equivalent and an corresponding points

The weighted density of a system or plane is the weight per unit area respectively. If N and n are the number of points of the same kind in a component set of the system and the plane respectively, the weighted densities are

٠Â

In the following table are given a number of important constants and expressions for each of the 14 lattices. From these by the use of the formulae reproduced below we can calculate the perpendicular distance between successive parallel planes and the densities of systems and planes.

Distance from origin to a plane fp+gq+hr+j=0

Distance between sucessive planes parallel to fl+gm+hn= 0

Volume of unit cell = $\frac{1}{\Delta}$ abc

Density of points in a system = $\frac{\Delta N}{\text{Sabc}}$ Density of points in a plane

$$= \frac{\delta \Delta n}{T(fVbc+gVca+hVab)}$$

•8	I	ttice	Sabo		T(fVbc+gVca+hVab)
_/	A	8			1 PL , Joh,
£. ;	1 ;	l abo	l-goos'	A+2008A008B008	$\frac{\mathbf{I}_{abc}}{\mathbf{E}_{ab}} = \frac{\mathbf{I}_{abc}}{\mathbf{E}_{abc}} = \frac{\mathbf{E}_{abc}}{\mathbf{E}_{abc}} = \mathbf{E}_{abc}$
<i>T</i> _m	1 1	l abcs	in A		abo $\int_{\overline{\Omega}}^{\overline{\Gamma}} \sin A + \frac{e^{+}h^{-}2eh}{b^{-}c^{-}bc} \cos A$
<i>T</i> ,	2	1 f+g even	_ ! # 1	e e e e e e e e e e e e e e e e e e e	1
1) ! } 1	½ f+g odd	t t		•
T.	1	1	(abo	$abc\sqrt{\frac{4}{a^t} + \frac{6}{b^t} + \frac{h^t}{c^t}}$
r.'	2 1	1 g+h even	1 · · · · · · · · · · · · · · · · · · ·	12 ° 13 m − 1 − 1 − 1 − 1 − 1 − 1 − 1 − 1 − 1 −	
1		g+h odd	t		\$1986 1
["	4	l f,g,h all	odd	•	
!		t otherwi	86	1	
Ţ*	2	1 two of f, even, one ½ otherwis	odd	· I Hoyan Swg	
T _e	1	1 1		i ab ^z	$ab^{2}\sqrt{\frac{t^{2}}{a^{2}}+\frac{p^{2}+h^{2}}{b^{2}}}$
Ţ,	1 1 2 1	l two of f, even, one	odd	T 11 1 1	T
<i>T.</i>	. 1	, ²		t t e ⁵	$a^{\epsilon}\sqrt{f^{\epsilon}+g^{\epsilon}+h^{\epsilon}}$
Ţ,	' 4	l f,g,hal	l odd	t (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	1 1 m
•	,	t de otherwi	.se	* * * * * * * * * * * * * * * * * * * *	
Ľ,	2	two of f,	odd	1 H	
	•	' ½ otherwi	.50	· 通過 等点	

We may consider $\int_{\mathcal{A}}$ to be expressed in terms of the three primitive vectors 1/3.0, 1/3.-1/3; 1/3, -1/3.0, 1/3; 1/3, 1/3, -1/3, 0 in which case its formula becomes /1a+mb+nc; $\Delta=1$ Sabc $=\frac{\sqrt{1-3\cos^2 A} + 2\cos^3 A}{2\cos^2 A}$ since here a=b=0

.81

= B = C

T(TWbc+gVca+hVab) = a (ffg+h)sinA, 1+2(gh+hf+fg)(cos A-cos A)

CHAPTER IX

X-Ray analysis of Crystals

(Elementary)

We may consider a crystal as in general a multiple

point system in which the place of the points is taken by
atoms of the different elements.

A crystal is always finite and is in general bounded by planes, but the number of atoms in even the smallest crystal is so great that these limitations need not be taken account of in considerations of internal structure.

The external symmetry of the forms of a crystal are often sufficient to determine which of the thirty-two classes of symmetry it belongs to, but cannot possibly reveal, except in class Q, which skeletal lattice and point system is the basis of their structure.

.1 Defraction of X-rays by crystals.

• 0

The distance between the atoms of a crystal is comparable to the wave length of X-rays which are diffracted by a crystal as from a three-dimensional grating.

Bragg has considered the effect as that of reflection from successive, equally-spaced, congruent planes of the crystal and obtains the simple grating formula

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

for maximum reflection where

d is the distance between successive planes

heta is the angle which the incident and reflected rays make with the plane

\(\lambda\) is the wave-length of the X-ray, and

n is an integer fixing the order of the reflection.

•11 If we keep λ constant and vary θ we obtain maxima of reflection when $\theta = \theta$, θ given by :

$$\sin \theta_i = \frac{n\lambda}{2d}$$

$$\sin \theta_{z} = \frac{2n\lambda}{2d}$$

$$\sin \theta_{\tau} \cdot \frac{\pi n\lambda}{2d}$$

on the other hand if we keep θ constant and vary λ , or what is the same thing, use "white" light, we have reflected at an angle θ rays of wave-length λ , λ , \dots , λ , given by:

$$\lambda_{r} = 2d \sin \theta$$

$$\lambda_{r} = \frac{2d}{2} \sin \theta$$

$$\lambda_{r} = \frac{2d}{2} \sin \theta$$

These two cases are the basis of the Bragg and Laue methods respectively.

Distribution of Energy among orders of Reflection.

. 2

.21

In general, however, the series of planes parallel to a given plane are not all congruent but consist of sets of different planes which are repeated regularly. Bragg has shown that the affect of this is analogous to that of the form of grating lines and leads to a different distribution of intensifty among the orders of reflections than that which would result from a series of congruent, equally-spaced planes.

In the latter case the intensity of the first, second, etc. orders falls off approximately as the inverse square of their order, i.e. in the ratio: 1, $\frac{1}{4}$, $\frac{1}{7}$

The intensity of a reflection of order n, due to a distribution of planes at distances d, d, d. from an initial plane, the whole being repeated at a distance d is given by

 $I_n = \frac{k}{n^2} (m_0 + m_1 \cos 2n\pi d/d + m_2 \cos 2n\pi d/d + ...)^{k}$

(m, sin 2nmd/d + m, sin 2nmd/d + ..)*

where m, m, represent the reflecting powers of the successive planes. m, is roughly proportional to the electronic density of the plane, i.e. to the weighted density, if to each atom of the plane we attribute the number of electrons associated with it, i.e. its atomic number. As the factor k is unknown we require relative and not absoute electron desities.

. 3 The Eragg I-ray Spectrometer Kethod.

In the Bragg method the crystal is mounted on a goniometer and a very fine beam of monochromates I-rays directed on to one face. The intensity of the reflected beam is measured by an ionisation chamber and a sensitive electroscope. The crystal and the ionisation chamber are so placed that the latter is always at twice the angular distance from the incident beam as the crystal face. The angles of reflection and the intensities of the first few order reflections from the face are measured.

•31 Determination of skeletal lattice

Such measurements for three faces of known indices suffice, fx if λ is known, to determine absolutely the ekeletal lattice of the system, i.e. to give both the nature of the lattice and the lengths and mutual angles of its reference vectors.

For by the formula given above we have $2d = \frac{n \lambda}{\sin \theta}$

also
$$d = \frac{\$ \text{Sabc}}{\$ (\$ \text{fVbc} + \$ \text{gVca} + \$ \text{hVab})}$$

*
$$\sqrt{\frac{1 - 2\cos^2 A + 2\cos A \cos B \cos C}{2 f^2 a^2 \sin^2 A + 22gh/ab(\cos A \cos B \cos C)}}$$

Now we know λ and $\sin\theta$; also from crystallographic data we know A B C and f g h.

Hence we have three equations of the type

•311

 $a_1x^2 + b_1y^2 + c_1x^2 + f_1yx + g_1xx + h_1xy + d_1 = 0$ $a_1x^2 + b_1y^2 + c_1x^2 + f_1yx + g_1xx + h_1xy + d_1 = 0$ $a_1x + b_1y + c_1x + f_1yx + g_1xx + h_1xy + d_2 = 0$ These are always soluble (in the most general case only by

elliptic functions). Thus a b c can always be found.

In practice, however, it is found that only the planes with simple indices give good reflections and these are generally used. In this case the equations above reduce to one or two terms each and the solution is correspondingly easy.

For the factor δ (see 8.52) which depends upon the lattice and upon the values of f g h, the latter are so chosen as to afford a criterion of the particular lattice. This may necessitate measurements from more than three planes.

Examples of planes which can be used for this criterion in the various crystal systems are given in the following table. For each lattice in a given system there will exist a ratio connecting the 1's of the various planes. A sufficient number of planes are chosen so that no two lattices of the same system have the same ratios of their d's.

```
.311 Triolinio
                sin A 1-1008 A+2 cos Acos Boos C; b sinB; c sinC
     lattice
       T
     Monoclinic d.,
                                           bc sin A
                       b sin A
                                  e sin A
                 la lb sin A c sin A
                  Orthorhombio
                  2a 2b 20 bo/ bic ca//o+a 2
                                             doll
      Tetragonal
                                             b/\2
                                 Ъ
                                 ½b ____
                                ā on
                      d ,,,
      Cubic
                                           a/\sqrt{3}
                                 a/\sqrt{2}
                      8
                                           a/ \sqrt{3}
                                B/2/2
                                _a/\[2 _ _ a/2\[3 _
                      <u>}</u>a
                      d ,,,,
                                a,01-1
       Rhombohedral
                                √3b/2
                                             ₽b
                       a
                                §3b/6 °
                                             <del>}</del>b
                      a/3
                                 d | 11-1-1
                       d ....
       Hexagonal
```

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•312 Thus in the case of rock salt NaCl a cubic crystal

 $d_{pp} : d_{pp} : d_{pp} : d_{pp} = 1:1/\sqrt{2}:2/\sqrt{3}$

The skeletal lattice is therefore \mathcal{L}' and $a = 2d_{100}$

It should be remembered in this connection, that except in the cubic system that the indices assigned to faces by crystallographers are not necessarily the same as those which are derived from the actual lattice of the crystal. As the former indices must necessarily be known first a lattice may be deduced which is not one of the 14 types. In such a case it is always possible to change the system of indices so as to reduce the lattice to a recognised form. This is well illustrated by the case of calcite, a crystal of class D for which Bragg found a face centered rhombohedral lattice with faces parallel to the form 101-1. If the lattice is taken as Γ_{ij} the indices of this form become 12-1-1.

•313 Screw axes

If the reflections from planes perpendicular to screw axes are measured the value of d will be h/k its normal value where h/k is the pitch of the screw. Since screw axes can only exist perpendicular to certain exemx planes it is always possible by choosing suitable planes to avoid any error on this score, and at the same time to determine the position and nature of all screw that exist.

Thus in the case of the diamond a cubic crystal containing only carbon atoms, $\mathbf{d}_{(0)}:\mathbf{d}_{(0$

32 Number of points in a component set

Having determined the lattice absolutely we can proceed to find the number of points in each component set by domparing the density of the crystal on the assumtion that there are N molecules per unit cell, with the observed density of the crystal.

The weight of each molecule is Lim where M is its molecular weight and m the weight of a hydrogen atom. We have therefore,

Density =
$$\frac{\Delta N \text{Mim}}{\text{Sabo}}$$
 or N = $\frac{\text{Sabo}}{\Delta \text{Mim}}$

= 2.96 = 3

- A

The formula of a molecule is in general written $X_X Y_y Z_z$... where x,y,z .. represent the numbers of atoms of x,y,z respectively in the molecule. The number of atoms of each kind per unit cell is accordingly Nx,Ny,Nz ... The number Nx when x is the least of x,y,z, ... is of the greatest importance in the eleucidation of crystal structure. It at once limits the number of classes and systems that the crystal may belong to. The crystal can belong to no system whose least subset has more points per unit cell t than Nx.

Thus in the case of quartz SiO_2 a crystal of the class D_3 Measurements show thath the lattice is I_k with a=5.38 × 10^{-1} cm.

From measurements of d_{1000} we have $d_{1000} = a/3$ and therefore there must be a screw axis. The basic system of quartz must therefore be one of D_3^3 D_3^4 D_3^5 D_3^6 with the Si atoms as a 3point sub group,

•33 Determination of class

The class of a crystal can usually be determined by crystallographic methods. In cases of crystals which only develop very simple forms the information these afford has to be supplemented by optical, electrical or other methods.

By the Bragg method it is possible to detect directly all symmetry relations except those that involve a centre of symmetry.

1331 If the class of the crystal is merchedral the orders of reflection from faces which belong to the same holohedral but not to the same merchedral forms will in general give different intensity distributions. The method fails when the two faces considered belong to forms whose faces are parallel to each other. For in this case the spacing of planes differ only in the two faces in that the sequence is inverse and as can be seen from the formula sufficient intensities.

Thus in the case of sinc blende Zn3 which is known to belon to class T_d there is no difference in the reflections from faces of the different forms 1,1,1 and -1,-1,-1, while for pyrites FeS_2 which belongs to class T_k the reflections from the faces 210 and 120 are totally distinct.

For the final determination of class in these doubtful cases we must have recourse to the methods of the next section.

.Z4 Determination of atomic positions

There are Nix atoms in a component set we have after determining the lattice, 3Nix unknowns to find, before the whole crystal is absolutely determined. We may have already found, however, a number of relations connecting these coordinates. If we know the symmetry class, the number of unknowns is reduced to 3Nix/k where k is the number of equivalent points in the class. If there is a sub set some of the unknowns may be exactly determined. We know what screw axes exist and from this and the information of the sub sets we to which may be able to limit the number of possible systems that the crystal may belong, to a very few. In this case, for each possible system the number of unknowns reduces to 3ix and may even from considerations of sub sets reduce to 0 in which case the crystal is completely determined. Whether such reductions may be effected or not the following method is applicable.

consider the series of planes parallel to fl+gm+hn=0. one each of passing through the points / (/), //x, //x, x). Their point densities are all equal to the dendity of points in the corresponding net of the skeletal lattice, while their electron densities are simply proportional to the atomic numbers of X, Y, Z,....

We have therefore for the value of the most the formula 4.21

$$\frac{S \Delta n_x}{T(fVbc+gVca+hVab)}$$
 whre n_x is the atomic number of an element X

The spacing of the planes is given by

$$d_{x_i}/d = J_{x_i}/\delta$$
 where $J_{x_i} = f \lambda_{x_i} + g \mu_{x_i} + h \nu_{x_i}$. Substituting in the formula

$$I_{A} = \frac{\delta \Delta k}{\text{rff}\{f \text{Vbc+gVca+hVab}\}} \left\{ \left\{ 2n \approx 2n \pi I_{A} / \delta \right\}^{2} + \left\{ 2n \approx 2n \pi I_{A} / \delta \right\}^{2} \right\}$$

If we are able to measure reflections from P planes and can obtain prorders of reflaction from each the r th plane we have Zp equations of this type. However as the equations are trancendental in/j, we cannot tell how many would be needed to find the 3N/x unknowns. The solution of a number of such equations is except in some simple cases extremely difficult and laborious. It should not prove difficult to construct a machine somewhat similar to a harmonic analyser, which would make / (/ pro) pass through all their possible values and select those which led to the observed values of xx reflection intensities. In view of the doubtful validity of the formula and the difficulties of exact measurements of intensities it is doubtful whether such a machine would justify itself at present. The method most used in practice is to reduce by means of the considerations of the last section the possible structures to a very few and beginning with the simplest and to compare the intensities calculated from them with those observed In this tentative method, analogies drawn from already eleucidated bragg was able to analyse rock salt, stivine, blende, diamond, fluorite and pyrites; all cubic crystals but of successively increasing complexity.

The Leve method

.41

-42

In this method a beam of "white" i.e. heterogeneous X-rays are allowed to fall on a properly oriented crystal and the rays reflected from the various planes are registered on a photographic plate placed behind the crystal.

The reflected rays are no longer white, but consist as was show in 9.12 of radiation made up of a series of wave lengths of different intensities.

The position of the spots on the photographic plate indicate merely the indices of the planes producing them, but as planes of the same form give spots of the same intensity, the nature of the symmetry of the crystal can be seen. The class however cannot in general be determined unambiguously, as for the reasons explained in 9.331 it is impossible to detect the absence of a centre of symmetry.

The intensities of the spots is an average offe of depending partly on the spacing and densities of the planes produceing them, partly on the wave length intensity distribution in
the incident beam. This renders interpretation very difficult,
but when the intensity distribution in the incident beam
contains only one maximum, it is possible to analyse some simple
crystals.

If the crystal is a lattice the spacing for all planes is even and the reflection for that plane which best reflects wave lengths near the maximum will be the most intense. The intensities of reflections from other planes will fall off re-gularly with the change of their indices. In the case of a crystal which is not a lattice however, the suppression of reflections by certain of the planes will cause the intensitions to vary irregularly with their indices and those irregularities may be used to discover their structure. Even in the simplest crystals this can only be done by trying various attractures with and comparing the apet intensities deduced from these observed.

In spite of these apparent limitations of the Loue method Ewald, Wycoff and others have devised improvements both on the experimental and theoretic sides by means of which remarkable results have been obtained.

as I know been tried, would be to take/Keue photographe with a source of miner homogeneous X rays of regularly varying wave length such as could be obtained for instance from a motating rock salt crystal illuminated by white rays. If the light were strictly homogeneous, the photographe would show no spots but the central one, for all but a certain number of wave lengths for which the reflections for certain planes would flach out. If such a method were to prove practicable as full results could be obtained from it as from the Brage method, for in this case the wave lengths being known, absolute measurements of length could be made, the absence of which, is the chief drawback of the Laue method.

•5 The Hull method

by Hull, and Debye and Scherrer. In this methed, not one, but also large number of crystals are used in the form of a metallic agaggregate or coarse powder spread on a plate or in the form of a thin cylinder. A beam of homogeneous X-rays is used. The crystals being arranged at random, there will always be a certain number that present some plane of the form f,g,h at such an angle to the incident beam that one of the orders of reflection occur and such reflected beabs are detected on a photographic plate or by an ionisation chamber.

- beam is 20 hence if we can find n . d is absolutely determined.

 It is often possible to pick out the orders of reflections due to the same plane on account of the simple relations between the sines of half the deflection angles.
- The great disadvantage of the Kull method is that we have no direct means of finding f,g,h. The intensities of a reflected beam is now proportional to that of the corresponding plane in the Bragg method multiplied by the number of faces in the form or in the case of a crystal not possessing a centre of symmetry, by twice this number; for it is obvious that the expectation of a suitably inclined face belonging to any form is proportional to the number of faces in the form, and that the intensity of of reflection is proportional to this expectation.

It can be seen that the Eull method leads to a similar but more complicated act of equations are the Bragg method and with many more unknowns. These equations are practically insoluble, and the method accordingly used in practice is to choose the st strongest of the scries of reflections as corresponding to the planes with simplest indices and to check the structure thus arrived at ty using it to predict the positions of the other 1 reflected beams.

or to substances which can only be obtained in the so called amorphous condition or in small(and imperfect crystals.

26.7

.6 Tabulation of results

The results obtained in an analysis of a crystal, whether or not they are complete can all be contained in the formula given an 9.34, the vectors a,b,c being also supposed known both in magnitude and in relative positions.

If however we assume the formula and also the symmetry elements of the 230 point systems as given in the tables in Ch VI all the results of an analysis may be given concisely as follows:

- .61 (i) The symbol of the skeletal lattice
 - (ii) the absolute dimensions both scalar and angular when necessa
 - (iii) the symbol of the point system. (Strictly speaking this includes the symbol of the lattice.)
 - (iv) the coordinates of one of each set of equivalent atoms stipulating the element.

From the set of of constants given under these heads we can calculate by the methods of Ch VII the position of exemy atom of each element in the crystal, and by the methods of Ch VIII the spacing and density of every set of parallel planes.

The number N of molecules of the substance per unit cell though included in the above deserves separate statement.

.62 In the following table these structural constants are given for a number of typical crystals which have been analysed by Bragg and others.

Name	Formula	N	Lt	Sm	Goordinates	Remarks
Rock salt	Nacl	1	r,"	0,5	Na C 0 0 C1 2 0 0	Other alkaline halides have similar structures
Zinc blen	đe ZnS	I	ŗ,	Td	Zn 0 0 0 S 1 1 1 1	
Diamond	c	2	<i>T</i> , '	OK	G ₁ 0 0 0	
Fluorite	CaF ₁	1	ţ'	0,5	Ca 0 0 0 F. 1 1 4	
Iron pyrites	FeS ₁	1	Ľ,	T4	Fe 000 3, 1-x x x	X has been variously given as 1/5 and 2/9
Cuprite	Cus	1	T _r	0,4	6 0 0 0 6 2 2 2 Cu 1 1	
TIN	Sn	Þ	$I_{\mathbf{t}}^{n}$	D.	Sn 0 0 0 Su ₂ ½ ½ 0	
Rhombic alkaline sulphate	sul HRSO s	1	Ţ,	Q 23	s 0 0 0	
Calcite	CaCO _s	1	V	D	Ca 0 0 0 0 2 0 0 0 ₃ 2 2x/3	Positions of atoms one given o-x/3 -x/3
Quartz	SiO _z	2	K	D ₃	S1, 0 2x/3	5 -x/3 -x/3 V V-A A-M .

In this table no lattice constants are given.

Appendix

A Suggestion for a natural, numerical denotation of Crystal Systems, Classes, Lattices and Point Systems.

There are many systems of denotation in use. Of these the most commonly known is that of Schoenflies which is used almost exclusively for internal structure. It is essentially a literal system and in it the letters correspond to various words used to describe the systems etc. This makes it easy to learn, but it suffers from several disadvantages.

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The basis of the system is the 32 Classes which are indicated by a capital letter with a suffix formed in general of a number and a letter. To denote 32 Classes by a triliteral symbol is unnecessary. The 14 lattices are all denoted by the letter Γ with suffixes and dashes: here again we have a triliteral system but this one has not even the advantages of the Class notation, as the manifest analogies between the different lattices are not shown by it. In the notation for point systems the method followed is to add to the Class symbol an index consisting of a serial number indicating the order of derivation of the system in the particular Class by Schoenflies method. This order cannot claim to be a natural order, and moreover the index gives no indication either of the skeletal lattice of the system or of its affinities to similar systems

in other Classes. It is practically impossible to remember the nature of any system denoted by its Schoenflies symbol, and references to the original derivation have constantly to be made.

The system suggested is free from these disadvantages. It is entirely numerical in character, making use of one other symbol only, the decimal point, which is used to mark off the . portion indicating the crystal system and class from that indicating the lattice and point system.

The symbol of a point system in its most general form consists of five numbers, two preceding the decimal point and three following. In holohedral systems, however, only one figure precedes the point and in some systems the number of figures after the decimal point often reduces to one or two. The significance of the figures is as follows:

The first digit from the left indicates the crystal system. The number denoting the 7 crystal systems are as follows:-

- O Triclinic
- L Monoclinic 2 Orthorhombic
- 3 Trigonal (Rhombohedral)
- 4 Tetragonal

The State State

- 6 Hexagonal
- Regular (Cubic)

It will be seen that except for the Monoclinic and Regular systems the number stands for the highest order of axes which the system possesses. We also have the convenient relation that any system is included as a special case by a system whose number is a factor of that of the first.

The second digit is used to distinguish the various Classes in each crystal system, so that we use a biliteral symbol for a Class.

The holohedral Classes have O for their second digit which can be omitted without causing confusion, thus giving the simplest symbol to the most commonly occurring Classes. The Holoaxial have 1 and so forth as shown in the table of Classes. All Classes containing only rotations of the first sort are designated by odd numbers; those with second sort rotations also by even numbers.

The first figure after the decimal point in conjunction with the first figure of all denotes the skeletal lattice. For normal lattices i.e. lattices with points only at the corner of rectangular parallelopipeda, this number is 0 (in the hexagonal and triclinal systems, as this is the only lattice, the figure 0 can be dropped). For centred lattices i.e. for lattices with points at the centres of rect. par. the number is 1. For face-centred lattices the number is 2. For the Orthorhombic lattice which has points at the centres of only one pair of faces of the rect. par. the number is 3. But besides these lattices, we may aften consider lattices that are not distinct from those, already denoted. These are To for which the number is 4 and To and To which are denoted by 4.2 and 4.3 respectively.

In the order of lattices .0, .1, .2, it is easily remembered that each has twice the number of points per unit per rect. par. as the one before it (except in the trigonal system).

The hexagonal lattice may be denoted either as 3.0 or 6.0 according as it occurs in trigonal or hexagonal systems. The notation for lattices is given in the table.

As far as possible the notation of the systems is arranged so that the numbers after the decimal point are the same in analogous systems, thus indicating in a large number of cases the sub-groupsof any system.

The notation for the 230 point systems is given in full with the corresponding Schoenflies symbols in the table below. It can be seen that in this method of denotation each symbol contains a considerable amount of information, While at the most employing five numbers (and in this not exceeding Schoenflies) it indicates all that the Schoenflies symbols indicate and more. L'oreover, it is comparatively easy to learn and with a little practice it is possible to obtain an idea of the actual configuration of all but the most complicated system by the mere inspection of its symbol.

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18.

CLASSES

			CLASSES				
System	HOLO HEDRAL	: '`), 		_Merche	d <u>ral</u>		
Triclinie	1 ,	Holo- hedral axial	Hemi- morphic	Alter- nating	Sphen-	'Tetarto-	Para- morphic
(Oblique)	1 C. O	C, 01	T — — — — T I	; ; ;	T 1 1	1 '1 1 1	r ! !
n onoclinic	C _{sk} 1	C ₂ 11	C, 12	r : :		T	
ortho-	Q 2	2 21	C _{2v} 22	; (r	
Tetra- 8 gonal	D ₄₄ 4	D ₊ 41	C ₄₀ 42	C 43	Q ₂ 44	C ₄ 45	C _{4A} 46
Trigonal (Rhombo- hedral)	D _M 3	D, 31	C, 32	C _{3i} 33		C ₅ 35	
Hexa- 8 gonal	D ₄₄ 6	D, 61	C 62	C3£ 63	D 64	C ₄ 65	6, 66
Regular (Cubic)	0, 8	0 81	T 82		T, 84	T 85	
			ATTICES				
Normal ;	F 0.0	T 1.0	T. 2.0	T. 4.0	T 8.0 ;	R 3.0	[6.0
Centred	8	7,1.1	T," 2.1 ;	Te' 4.1 ;	元"8.1 :	Th 3.1 !	
p Face centred				F, 4.2;			
l Face : centred :			[, 2.3]	Fee 4.3	Alŝ	ο Γ' _{ε β} 2.4	

					FOIRT	515TE							
Cl	888	• 100 -	1						a	•		14 48 * 7.2	
C,	01.		1.	.0									
Cį	0.		1.	.0			.,			-		and the second of the second of	
C ₂	11.		1.	.00	٤ .01	3 .1	D						entropies and
C _s	12.		ı,	.00	2 .01	3 .1	.0	4 .1	i.	-			
C _{zk}	2.			.000 .001	2 .010 5 .011	3 .1 6 .1							
G _k		20 18 11	.30	22 .11 19 .21	3 .02 21 .12 13 .32	5 .03	1	.04		6 .06		3 .08 10	.010
Q	21.		1 8 7 6	.00 .10 .20	2 5	.01		3	.08	.02	4 03 9 .13		
Q _k	2.		1 2 4 3	.000 .001 .002	5 7 6	.010 .011		9 13 10 14	.020 .022 .023		15 .03 16 .03	. 40	
			25 ₄ 26 23 24	.100 .101 .200 .203		:		12	.025		27 .136 28 .13		
<u>.</u>			19 21 22 20	.300 .301 .302 .303	17	.310			: i				

POINT SYSTEMS

In the first of each double column is given the Schonfleis serial index of the point system; in the second the decimal part of the proposed notation, the whole number part being given under the head of class.

	• • • • • • • • • • • • • • • • • • • •					
Class						
C ₄ 45.	 		3 .02	4 .03	5 .10	6 .11
C ₄ 43	1.00		-		2 .20	
C _{1A} 46	1 .00 3 .00	00	2 .020 4 .022		5 .100	6 .112
C, 42.	1 .00 5 .00 2 .00	1	3 .020 7 .021		9 .100	11 .111
	6 .00	3	4 .022 8 .023		10 .102	12 .113
D ₄ 41.	1 .00 2 .00		5 .020 6 .022	7 .030 8 .032	9 .100	10 .112
D _{4A} 4.	1 .00 2 .00 3 .00 4 .00 201 5 .00 6 .00 7 .00	OD 02 03 20 21	10 .0200 9 .0201 12 .0202 11 .0203 14 .0220 13 .0221 16 .0222		17 .1000 18 .1001	
D _{2/} 44.	1 .000 2 .000 3 .020	9 .100 2 10 .102	15 .0223 11 .200 12 ,202	5 .300 6 .302 7 .320		19 .1102 20 .1103
	4 .021	2		8 .322		
T 85.	1 .00 3 .10 2 .20			4 .03 5 .13		
T, 82.	1 .000 2 .003 5 .100 \$.200 4 .203	3		6 .030		
T, 84	1 .000 4 .001 8 .100 2 .200 5 .201			6 .131		
					* 1 2 2 **	i Nord transcondent

X .

	Cla	88.												
• • •	0	81.	12 534	.000 .002 .100 .200 .202					6 7 8	.031 .033 .130				
	0,	8. 1	123495678	.0000 .0003 .0020 .0023 .1000 .2000 .2001 .2022 .2023					10	.1300)			Spinos Control
	c,	35.	1	.00		2	.01	VARIO CELE	3	.02		4	.10	
	C _{st}	33.	1	•0						ì		2	.1	
	C,	32.	1 2	.00		3 4	.01			i		5 £6	.10	
	D,	31.	2	.00		4 3	.01		6 5	.02 22.		7	.10	
	D _{s.}	3.	2 3 4	.00 .01 .20							•	5 6	.10	
	C,	65.	1	:00	2	.1	4.	.2	14	.3	5	.4	8	.5
	Cost	66.	1	.0					2	.3				
	C3,6	63.	1	.0				İ			/ Mar 40.00			
	D, /	64.	1 3	.00					2 4	.03		•		
	C	62.	1 3	.00					2 4	.03			25 M 100 11 W	
	D6	61.	1	.00	2	.1	4	.2	6	•3	5	.4	3	•5
	D	6.	1 2	.00			,		3 4	.30				
•							l							