A STUDY IN CRYSTALLOGRAPHY

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PREFACE

The following study of Crystallography is by no means a complete work, but merely an introduction to the determination and classification of possible crystal structures in three-dimensional space. I will not try to outline my work here, or attempt to list its applications but I do feel that it is applicable to quite a variety of studies and a basis for further research.

My main attempt in the writing of this has been to give fellow undergraduate mathematics majors a brief introduction to one of the possible areas of study toward which their work may lead them, and to provide a basis for the work of solid state physics students. Further research in this field also leads to the study of crystal formations found in nature, as are used by chemists, geologists and others, and to the study of crystals by x-ray diffraction methods used extensively by physicists.

In preparation for this work I have reviewed and applied much of the work in abstract and linear algebra, the geometry of symmetries and vector spaces. I will at times presuppose a general knowledge in these fields. Further information on these basics can be obtained from the book Geometry and Symmetry by Paul B. Yale[1], to whom I am very grateful for his informative and concise approach to the

[1] Paul B. Yale, Geometry and Symmetry (San Francisco, Holden-Day, Inc., 1968).

field of Crystallography. Another valuable reference is the International Tables for X-Ray Crystallography[2] which I have used extensively for detailed information and standard symbols used in crystallographic work.

[2] International Tables for X-Ray Crystallography, ed. by Norman F. M. Henry and Kathleen Lonsdale (Birmingham, England, The Kynoch Press, 1952), vol. I.

Chapter I

Introduction

Section 1. - What is Crystallography?

Crystallography is the study of the structure, form, properties, and classification of crystals. From a non-mathematical point of view, a crystal may be defined as a structure in 3-dimensional space which is made up of a regular repetition of identical structural units, forming parallelepipeds. In order to understand this concept of 3-dimensional crystals we may look at their equivalent structures, called tiles, in 2-dimensions. Here we again have a regular repetition of identical units which form parallelograms, and in both of these cases, in the plane and in space, the parallelograms or parallelepipeds fill the plane or space, respectively. That is, the structures all share sides and there is no space between them and no overlapping.

To determine the possible tiling patterns or crystal structures that may exist we will slightly alter the wording of these definitions so that we will be talking about points in the plane or in space rather than actual structural units. Then we can apply our knowledge in mathematics to determine the crystal structures, no matter what the units such as atoms, molecules, or whatever which the tile or crystal has in nature. Thus we will now be speaking of

tiles or crystals as having equivalent points rather than identical structural units. Figure 1-1 shows a tiling pattern in 2-dimensions and the equivalent points within two parallelograms are shown.

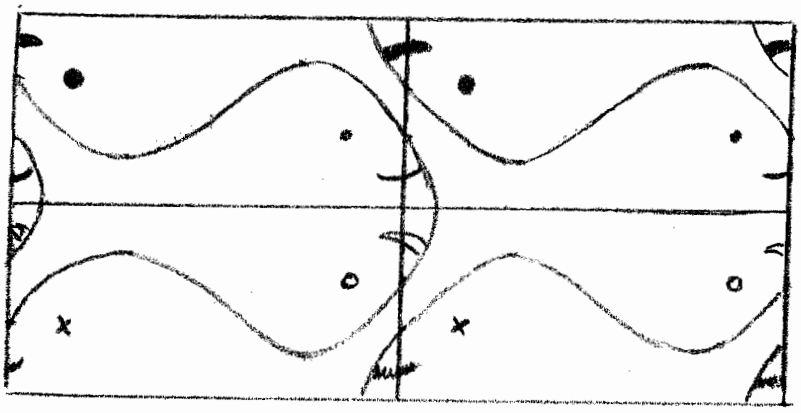


Figure 1-1

Note also in this figure that the tiles completely fill the plane with no overlapping, and when we talk about crystals they will completely fill all of space in this same manner.

In mathematical terms we can now defime a crystal structure as follows:

A <u>crystal</u> in 3-dimensional space consists of the union of a collection of bounded sets with congruent components, that are space-filling, and intersect only at their boundaries. That is, a crystal is the union of a collection of compact, closed, and bounded sets.

Section 2. - Beginning the Classification of Crystals

Now we may begin to classify crystals, which we know exist, of course, and are therefore worthwhile studying. Given any crystal we know that it is made up of finite parallelepipeds, and thus may be examined from the standpoint of the finite number of positions and directions which the points of each parallelepiped may be oriented in. We are interested first in the distances between any two equivalent points in the structure, and for simplicity I will explain these distances in terms of vectors that are determined by this distance between the points. Then we will use these vectors to define a <u>lattice</u>, a net-work of parallelepipeds. Thus a 3-dimensional lattice is an infinite array of points such that each point has the same environment in the same orientation. A single lattice structure is called a <u>unit cell</u> and it is chosen for each crystal as determined by the basic unit parallelepiped which is repeated in the crystal. Three vectors define a unit cell in 3-dimensions, and they form the edges of the parallelepiped. We shall be calling these vectors $\vec{a}$,$\vec{b}$, and $\vec{c}$, and their length and direction will be determined differently for each case that we study. The angles between the vectors are; α, the angle between $\vec{b}$ and $\vec{c}$, β, the angle between $\vec{c}$ and $\vec{a}$, and γ, the angle between $\vec{a}$ and $\vec{b}$. These lattices that we will define are called Bravais lattices,

after their founder, and may be taken as arrangements of points in real space, the repeat distance between the points in any particular direction being proportional, in any particular case, to the corresponding repeat distance in the real crystal under study, and thus we have found our basic unit of classification of all crystals.

The idea of lattices may be approached from a more mathematical standpoint also. Intuitively vectors correspond to translations of the entire space from one position to another. For example, the translation corresponding to a vector of length 1 in the positive x-direction of a real plane is a translation which moves each point of space 1 unit in the positive x-direction. Therefore a more convenient formulation of the lattice concept is as follows:

Definition: A lattice group, L, is a nontrivial, discrete subgroup of T, the group of translations, i.e. L is a lattice group if $L \neq \{1\}$, L is discrete, and every element of L is a translation.

Note: In our study of lattices that follows we will be looking at the lattice as a subgroup of the set of all 3-dimensional vectors and also as a group of translations.

Having now introduced our basic unit of classification, the Bravais lattice, under which we shall place crystals into seven systems, we find that we can break down this classification into 230 categories, called space groups.

The translations which are the basis of the lattices relate one part of the crystal structure to another part, but there are usually (except in the most trivial cases) other symmetries of the crystal system which are not translations. These symmetries include rotations, inversions, and reflections, and products of these with translations, i.e. glide reflections and screw displacements.

Definition: A crystallographic space group G is the group of all symmetries of a crystal structure. The subgroup $G \cap T$, of all translations in G is a 3-dimensional lattice group.

It will then be convenient to classify crystals according to the complexity of the non-translational aspect of the space group. This aspect is referred to as the point group.

Definition: A crystallographic point group is a subgroup of the group of symmetries which leaves a point X and some 3-dimensional lattice containing X fixed.

We will find later that there are 32 such point groups by which all crystals may be categorized. The symmetries that will be included in these point groups are rotations about a line, reflections in a plane, and inversions in a point, and we can now begin the classification by finding the restrictions that are placed on some of these symmetries.

For each crystal we have noted that we may choose 3 vectors $\vec{a}, \vec{b}$, and $\vec{c}$ that are the axes of a unit cell for

that crystal. We will also have an axis of rotation for each crystal, and by determining our choices of vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$ with respect to this axis of rotation we can restrict the possible rotational symmetries of a crystal.

Lemma 1-1. If l is the axis of rotation ρ, then we can choose vectors parallel and perpendicular to l.

Proof: Suppose l is our n-fold axis of rotation.

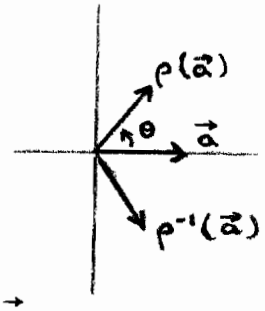
1. Choose a point p on l and a vector $\vec{d} \ni p \in \vec{d}$ and $\vec{d} \not\perp l$.
   Then we know that $\sum_{k=0}^{n-1} \rho^k(\vec{d})$ is parallel to l.
   $\therefore \exists$ vectors parallel to l.
   Let $\vec{c}$ be the shortest vector parallel to l.
2. Now let $\vec{d} \not\parallel l$.
   $\sum_{k=0}^{n-1} \rho^k(\vec{d}) - nd \perp l$.
   $\therefore \exists$ vectors, $\vec{a}$ and $\vec{b} \perp l$.

Thus we now can choose our three vectors $\vec{a}, \vec{b}$, and $\vec{c}$, with $\vec{c} \parallel l$, and $\vec{a}, \vec{b} \perp \vec{c}$, and we can see that any rotational restrictions will be dependent of the angle of rotation of $\vec{a}$ or $\vec{b}$ about $\vec{c}$. In other words, we may now view our crystal in two dimensions which makes the following proof easier.

Theorem 1-2. Crystallographic Restriction. Let ρ be a non-trivial rotation in a crystallographic point group. The order of ρ is 2, 3, 4, or 6.

Proof: Choose $\vec{a}$ to be the minimal vector to an equivalent point in our crystal.

Look at $\rho(\vec{a})$ and $\rho^{-1}(\vec{a})$, Figure 1-2. These vectors will be the same length as $\vec{a}$ and any combinations of them must be of the same length or an integer multiple of this length since each vector in the crystal must take us to another equivalent point in it.



Consider $\rho(\vec{a}) + \rho^{-1}(\vec{a}) - \vec{a}$

$\rho(\vec{a}) = a(\vec{i}\cos\theta + \vec{j}\sin\theta)$

$\rho^{-1}(\vec{a}) = a(\vec{i}\cos\theta - \vec{j}\sin\theta)$

$\vec{a} = a\vec{i}$

$\therefore \rho(\vec{a}) + \rho^{-1}(\vec{a}) - \vec{a} = (2\cos\theta - 1)\vec{a}$

By our above statements of reason we know that $2\cos\theta - 1$ must be either 0 or an integer.

Case 1. $\theta = 60°$

Then $2\cos\theta - 1 = 0 \Rightarrow$ there may be a rotation of order 6.

Case 2. $\theta < 60°$

$2\cos\theta - 1 > 0 \Rightarrow$ this is impossible and thus the greatest order of rotation that we may have is 6.

Case 3. $\theta = 72°$

$2\cos\theta - 1$ is a fraction, thus ρ^5 is impossible.

Case 4. $\theta = 90°$

$2\cos\theta - 1 = 1 \Rightarrow \rho^4$ is possible.

Cases 5. & 6. $2(60°) = 120°$ and $2(90°) = 180° \Rightarrow \rho^2$ and ρ^3 are possible.

We now may conclude that for any ρ $\ni$ $n\rho = 2\pi$, $n = 2,3,4,$ or 6, and this theorem will now become one of our basic tools for further study.

Section 3. - Overall Picture

In summary, our work from this point on will be to try to classify all possible space groups. We can view the analysis in the following way:

Each crystal structure determines a unique space group, which determines a unique point group. There are 32 point groups in all, which can be classified into 7 crystal systems, for each of which there is at least one type of lattice. Indeed the lattices can be classified into 14 types called the Bravais lattices. By combining each point group with all of its associated lattices 230 different space groups can be realized. Table 1.1 shows the breakdown into these different groups.

Table 1.1

Crystal Systems	Number of lattices	Number of point groups	Number of space groups
Triclinic	1	2	2
Monoclinic	2	3	13
Orthorhombic	4	3	59
Tetragonal	2	7	68
Cubic	3	5	25
Trigonal	1	5	27
Hexagonal	1	7	36
Totals: 7	14 *	32	230

*

Chapter II

Forming the Bravais Lattices

We have noticed in the preceding chapter that each crystal structure determines a space group, which in turn determines a lattice group and a point group. In this chapter we attempt to classify the structures according to the existence of certain symmetries in their point groups. The restrictions on rotations that we have found will be the basis for our choices of what our point groups will look like. I note at this point that our choice of vectors for axes for each group may not necessarily be the natural ones which would seem to arise, but we will be selecting the preferred or conventional ones which make the work easier and more applicable.

Determining the lattices :

Suppose that our crystal structure under study has point group G and lattice group L :

CASE I. G contains a 6-fold rotation ρ with axis l.

The lattice will be called the hexagonal lattice and will be constructed as follows:

Let $\vec{c}$ be the shortest vector parallel to l, and we will consider it to be in the z-axis direction.

$\vec{a}$ will be the shortest vector perpendicular to l, call it the x-axis direction.

$\vec{b} = \rho^2(\vec{a}) \Rightarrow \rho(\vec{a}) = \vec{a} + \vec{b}$ and $\rho(\vec{b}) = -\vec{a}$ as shown in Figure 2-1.

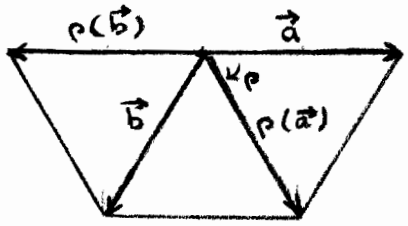


Figure 2-1

Note: We choose ρ^2 as the angle γ between $\vec{a}$ and $\vec{b}$ by convention. This convention being that the angle be greater than 90°. As we will see later, this convention makes it possible to use this primitive hexagonal lattice in another system, the trigonal system, where there is a 3-fold rotation axis.

These vectors determine the primitive hexagonal lattice of the Hexagonal system as shown in Figure 2-2, with lattice points at the vertices of the figure.

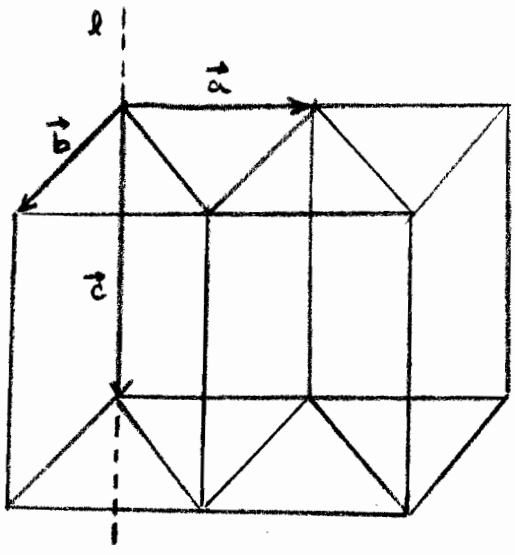


Figure 2-2

Angles

$\gamma(\vec{a} \wedge \vec{b}) = 120°$

$\alpha(\vec{b} \wedge \vec{c}) = 90°$

$\beta(\vec{c} \wedge \vec{a}) = 90°$

Before completing our examination of this case we must consider the possibility of points on a lattice other than at the vertices. Thus far we have assumed that the points at the vertices are the only ones, but since we restrict our choice of vectors for axes there is the possibility that other points exist that we have missed. The existence of such points produces a condition which is called centering for reasons which we shall soon discover, and we shall find that there are only certain types of centering which can exist.

Lemma 1: Suppose that L is the full lattice and P is the primitive lattice generated by $\vec{a},\vec{b}$, and $\vec{c}$. Then if there is some $\vec{d}$ in L which is not in P, $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ where p,q, and r are rational numbers, and furthermore, we may assume the following:

$$0 \leq p < 1 \ , \quad 0 \leq q < 1 \ , \quad \text{and} \quad 0 \leq r < 1$$

Proof: $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ for some real numbers p,q, and r, since $\vec{a},\vec{b}$, and $\vec{c}$ are independent of each other.

If any of the coefficients is irrational then there are an infinite number of vectors in L which are contained in the unit cell.

But this contradicts the discreteness* of L.

If $[p] = l$, $[q] = m$, $[r] = n$, ($[\ ]$ denotes the greatest integer) replace $\vec{d}$ by

* If the term discreteness is unfamiliar I suggest reviewing its definition in Yale (f.n.1) or in most any geometry text.

$$\vec{d} - l\vec{a} - m\vec{b} - n\vec{c}$$

and we can easily see that this equation must be equal to zero or less than 1 $\Rightarrow$ $0 \leq p < 1$, $0 \leq r < 1$, and $0 \leq q < 1$.

The types of centering that we will be finding are as follows:

1. L is said to be body-centered, I, if it contains $\vec{a}/2 + \vec{b}/2 + \vec{c}/2$, that is, a point at the center of each cell as well as at the vertices.

2. L is a face-centered lattice, F, if it contains a point at the center of each face besides those at the vertices.

3. L is an end-centered lattice, A,B, or C, if it contains a pair of points at the center of opposite faces besides the vertex points. A denotes an end-centered lattice with points on the x-plane, B, for points on the y-plane, and C, on the z-plane.

Returning to the Hexagonal system, we must now check for the centering possibilities so that we can find all the Bravais lattices.

Suppose $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ is any element of L which is not in P.

We note first that no two of p,q, or r can be zero since each of $\vec{a},\vec{b}$, and $\vec{c}$ is the shortest vector of L in its own direction.

Case 1. Now suppose r = 0

$\vec{d} = p\vec{a} + q\vec{b} \in L$

Then say $p = \frac{p_1}{p_2}$ and $q = \frac{q_1}{q_2}$ in lowest terms

$q_2\vec{d} = \frac{q_2 p_1}{p_2}\vec{a} + q_1\vec{b}$

Since $q_2\vec{d}$ and $q_1\vec{b} \in L$

$\frac{q_2 p_1}{p_2}\vec{a} \in L$, hence $\frac{q_2 p_1}{p_2} \in Z$ and $\frac{q_2 p_1}{p_2}\vec{a} = q_2\vec{d} - q_1\vec{b}$

p_1 and p_2 have no common factors, therefore p_2 divides q_2 which signifies the following:

Every vector or the type $p\vec{a} + q\vec{b}$ with 0 p 1 and 0 q 1 is shorter than $\vec{a}$ and because we have chosen $\vec{a}$ to be the shortest perpendicular to $\vec{c}$, the only possibility is p = q = 0 which we have excluded.

Case 2. Suppose either p = 0 or q = 0.

Assume p = 0, then by our earlier remark, neither q nor r equal zero.

Hence $\vec{d} = q\vec{b} + r\vec{c}$ where 0 r 1 and 0 q 1

$\vec{d} - p^3\vec{d} = (q\vec{b} + r\vec{c}) - (-q\vec{b} + r\vec{c}) = (2q)\vec{b}$

$\therefore q = 1/2$

$\vec{d} + p^3\vec{d} = (q\vec{b} + r\vec{c}) + (-q\vec{b} + r\vec{c}) = (2r)\vec{c}$

$\therefore r = 1/2$

Hence $\vec{d} - p\vec{d} = (q\vec{b} + r\vec{c}) + (q\vec{a} - r\vec{c}) = q\vec{b} + q\vec{a} = \frac{\vec{b}}{2} + \frac{\vec{a}}{2}$

But this is impossible as we have shown in Case 1.

Case 3. Suppose none of p,q, or r = 0

$\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ and $0 < p < 1$, $0 < q < 1$, and $0 < r < 1$

$\vec{d} + \rho^3\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} - \rho^3\vec{d} = 2p\vec{a} + 2q\vec{b}$

By Case 2, 2p and 2q $\in Z$, hance $p = 1/2$ and $q = 1/2$

$\therefore \vec{d} = 1/2(\vec{a} + \vec{b} + \vec{c})$

Now since $\rho(\vec{a}) = \vec{a} + \vec{b}$ and $\rho(\vec{b}) = -\vec{a}$

$\vec{d} - \rho(\vec{d}) = 1/2(\vec{a} + \vec{b} + \vec{c}) - 1/2(\vec{a} + \vec{b} - \vec{a} + e)$

$= 1/2\vec{a}$ is in L.

But this is a contradiction of $\vec{a}$ as our shortest vector.

CASE II. G contains a 4-fold rotation ρ with axis 1, but no 3-fold rotation.

The primitive lattice will be called the tetragonal lattice of the Tetragonal System, and we will construct it as follows:

Choose $\vec{c}$ to be the shortest vector parallel to 1

$\vec{a}$ is the shortest vector perpendicular to 1

$\vec{b} = \rho(\vec{a}) \Rightarrow \rho(\vec{b}) = -\vec{a}$

Thus we have our primitive tetragonal lattice (Figure 2-3) with $a = b \neq c$, and $\alpha = \beta = \gamma = 90$

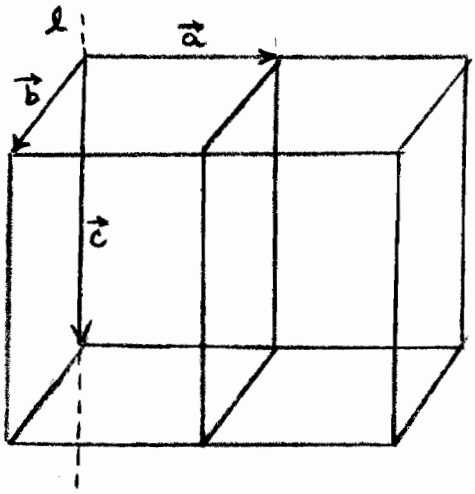


Figure 2-3

We must now consider the possibilities for centering. Suppose $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c} \in L$ but $\notin P$. We need consider only the same cases as in Case I since $\vec{a}, \vec{b}$, and $\vec{c}$ are the shortest vectors in their own directions once again.

Case 1. Suppose $r = 0$

$\vec{d} = p\vec{a} + q\vec{b} \in L$

Letting $p = \frac{p_1}{p_2}$ and $q = \frac{q_1}{q_2}$ in lowest terms as in Case I

we have $q_2\vec{d} = \frac{q_2 p_1}{p_2}\vec{a} + q_1\vec{}$

$\therefore \quad \frac{q_2 p_1}{p_2} \vec{a} \in L \Rightarrow \frac{q_2 p_1}{p_2} \in Z$ and p_2 divides q_2

Since $0 \leq p < 1$ and $0 \leq q < 1$ this case is impossible to have since either $\vec{d}$ or $\vec{a} + \vec{b} - \vec{d}$ is shorter than $\vec{a}$.

Case 2. Suppose either $p = 0$ or $q = 0$

Assume $q = 0$ and $p \neq 0$

$\vec{d} = p\vec{a} + r\vec{c}$ and since $r \neq 0$, $0 < r < 1$ and $0 < p < 1$

$\rho^2\vec{d} = -p\vec{a} + r\vec{c}$

$\therefore \quad \vec{d} - \rho^2\vec{d} = 2p\vec{a} \Rightarrow p = 1/2$

$\vec{d} + \rho^2\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} - \rho\vec{d} = p\vec{a} - p\vec{b}$ but this is impossible by Case 1.

Case 3. None of p,q, or r are zero

$\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ and $0 < p < 1$, $0 < q < 1$, and $0 < r < 1$

$\vec{d} + \rho^2\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} - \rho^2\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

In fact this vector could be in L, yielding a body-centered tetragonal lattice, I. Now we have 2 more Bravais lattices, the primitive lattice P, and the body-centered lattice, I, both of the Tetragonal system.

CASE III. G contains a 3-fold rotation σ with axis k, and a 4-fold rotation ρ with axis l, but no 6-fold rotation. l and k cannot be parallel or perpendicular since otherwise $\sigma\rho$ would be a 12-fold rotation.

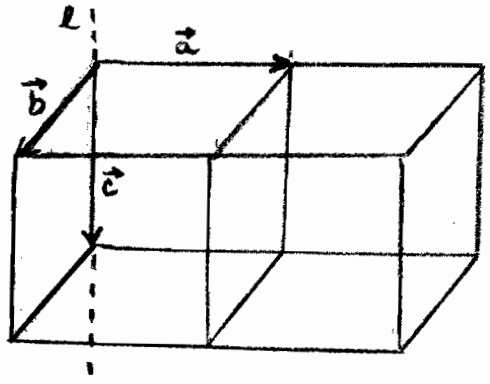
Our basic lattice will be called the primitive cubic lattice of the Cubic System, and will be constructed as follows:

$\vec{c}$ is the shortest vector parallel to l

$\vec{a} = \sigma\vec{c}$

$\vec{b} = \sigma^2\vec{c} = \sigma\vec{a}$

By means of a very complicated proof, it can be shown that $\alpha = \beta = \gamma = 90$ but we will simply assume this fact. Thus the unit cell of the primitive lattice is a cubic prism, with a = b = c, placing the 3-fold axis k along a diagonal. Figure 2-4 shows the primitive cubic lattice.



We may assume:

$\sigma\vec{a} = \vec{b}$
$\sigma\vec{b} = \vec{c}$ and $\rho\vec{a} = \vec{b}$
$\sigma\vec{c} = \vec{a}$ $\rho\vec{b} = -\vec{a}$

Figure 2-4

Again we must check for centering possibilities.

Let $\vec{a} = p\vec{a} + q\vec{b} + r\vec{c}$ be $\in$ L but $\notin$ P.

Case 1. Suppose any two of p,q, and r equal zero.

a. If $p = q = 0$ then $\vec{d} = r\vec{c}$ with $0 \leq r \leq 1$

Since $\vec{c}$ is the shortest vectoe in its direction r must be either 0 or 1. Thus this vector produces no new points.

b. Assume $q = r = 0$, then $\vec{d} = p\vec{a}$ with $0 \leq p \leq 1$

But $\sigma^2(\vec{d}) = p\vec{c}$ and by Case 1. we have shown that $p = 0$ or 1, thus there is nothing new.

Case 2. Suppose $r = 0$, $q = 0$, or $p = 0$.

Assume $r = 0$. Then $\vec{d} = p\vec{a} + q\vec{b} \in L$.

$\sigma\vec{d} = p\vec{b} + q\vec{c}$ and $\sigma^2\vec{d} = p\vec{c} + q\vec{a}$ which are vectors of length d on the other two planes.

$\vec{d} - \rho^2\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

Hence we have new lattice points at the center of each of the faces of the cube besides the vertex points forming the face-centered cubic lattice, F.

Case 3. Suppose none of p,q, or r are zero.

$\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$ and $0 < p < 1$, $0 < q < 1$, and $0 < r < 1$

$\vec{d} + \rho^2\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} - \rho^2\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

This means that we have a new vector $\vec{d} = \frac{\vec{a}}{2} + \frac{\vec{b}}{2} + \frac{\vec{c}}{2}$, and in fact this vector is in L, yielding the body-centered lattice, F, and the body-centered lattice, I.

We now have found three Bravais lattices of the Cubic System, the primitive lattice, P, the face-centered lattice, F, and the body-centered lattice, I.

CASE IV. G contains a 3-fold rotation, ρ, and reflections are parallel or perpendicular to the rotation axis 1. There are no 4- or 6-fold rotations.

In this particular case we will form two primitive lattices of the Trigonal System, the reason for this being explained as we proceed.

1. The shortest vector is parallel to 1.

   Call this vector $\vec{c}$, as we have been doing.

   $\vec{a}$ will be the shortest vector perpendicular to $\vec{c}$

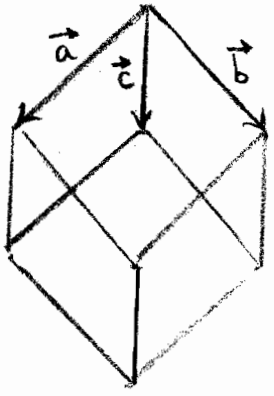
   $\vec{b} = \rho\vec{a}$

   What we have formed is the primitive hexagonal lattice as shown in Figure 2-2. Bear in mind that we may always form this lattice when G has the above properties, but the second case we will examine produces a smaller cell, and thus is more convenient to use in the situations when it is possible.

2. This case is used when the shortest vector is neither parallel or perpendicular to 1.

   Call this vector $\vec{a}$, and let $\vec{b} = \rho(\vec{a})$ and $\vec{c} = \rho^2(\vec{a}) = \rho(\vec{b})$

   We have now formed the rhombohedral lattice, R, as in Figure 2-5.



$|a| = |b| = |c|$

$\alpha = \beta = \gamma \neq 90°$

Figure 2-5

Centering will not exist in the hexagonal lattice as we proved in Case I, but we must check the rhombohedral lattice.

Suppose $\vec{d} \in L$, and $\notin P$. Clearly $|\vec{d}|$ must be greater than $|\vec{a}|$ since $\vec{a}$ is the shortest vector to a point.

If $\vec{d}$ is any vector besides the vector to the center of the cell we can clearly see that it will be closer to one vertex than $\vec{a}$, thus we need only consider the center point.

(a.) If the vector $\vec{d} = \frac{\vec{a}}{2} + \frac{\vec{b}}{2} + \frac{\vec{c}}{2}$ is shorter than $\vec{a}$, then we are in a position to pick the hexagonal lattice, thus there is no centering.

(b.) If $\vec{d}$ is longer than $\vec{a}$, then it is closer than $|\vec{a}|$ to another of the vertices, which would again put us in a position to choose a hexagonal lattice.

Thus in the Trigonal System we have only primitive lattices, the hexagonal lattice, P or the rhombohedral lattice, R.

CASE V. G contains no 3- or 4-fold rotations, but it does contain two perpendicular axes, of rotations of order 2, or reflections.

Note: Two perpendicular axes produce a third 2-fold or reflection axis perpendicular to these.

Figure 2-6 shows the primitive orthorhombic lattice of the Orthorhombic system, and it is constructed as follows:

$\vec{a}, \vec{b}$, and $\vec{c}$ are the shortest vectors parallel to the axes. Thus $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90$

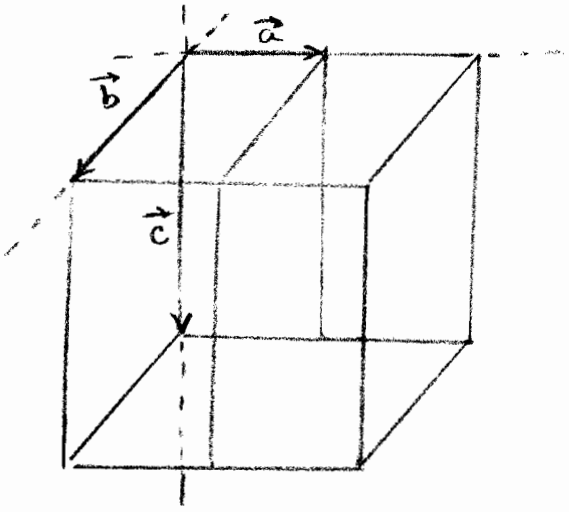


Figure 2-6

For centering consider $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c} \in L, \notin P$.

Case 1. Suppose $r = 0$ and we are considering 2-fold rotations.

A. $\vec{d} = p\vec{a} + q\vec{b}$ and we will choose the direction of $\vec{c}$ to be along the axis of rotation .

$\rho\vec{d} = -p\vec{a} - q\vec{b}$

$\vec{d} - \rho\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

If σ is the rotation with its axis in the direction of $\vec{a}$, and θ, the rotation with axis along $\vec{b}$ we find the following:

$\sigma\vec{d} = p\vec{a} - q\vec{b}$ and $\theta(\vec{d}) = -p\vec{a} + q\vec{b}$ which make p and q equal to 1/2 again, and produce only points at the center of the plane determined by $\vec{a}$ and $\vec{b}$.

Thus we may have an end-centered orthorhombic lattice, C.

The same procedure can be followed for p = 0 and q = 0 as for r = 0 and we will find the ecd-centered lattices A and B respectively. These lattices are of the same type, depending only upon which face our point is centered in, thus they produce only one new category of lattice called either A,B, or C.

B. Now consider a reflection $m \perp c$ and r = 0, p = 0, or q = 0

Assume r = 0

$\vec{d} = p\vec{a} + q\vec{b}$

$m\vec{d} = p\vec{a} + q\vec{b} = \vec{d}$

$\vec{d} + m\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

If n is the reflection $\perp \vec{a}$, and k, the reflection $\perp \vec{b}$, we have

$n\vec{d} = -p\vec{a} + q\vec{b}$ and $k\vec{d} = p\vec{a} - q\vec{b}$.

$\vec{d} + n\vec{d} = 2q\vec{b}$, $\vec{d} - n\vec{d} = 2p\vec{a} \Rightarrow q = 1/2$ and $p = 1/2$

$\vec{d} + k\vec{d} = 2p\vec{a}$, $\vec{d} - k\vec{d} = 2q\vec{b} \Rightarrow q = 1/2$ and $p = 1/2$

$\therefore$ We have again produced the end-centered lattice C, and by similar work with p and q and the reflection we get A and C.

Case 2. Suppose we have any two of the following vectors:

$\vec{d} = p\vec{a} + q\vec{b}$, $\vec{f} = q\vec{b} + r\vec{c}$, or $\vec{g} = p\vec{a} + r\vec{c}$

By Case 1, A and B we know that p,q, and r = 1/2

Assume $\vec{d}$ and $\vec{f} \in L$ but $\notin P$

$\vec{d} + \vec{f} = p\vec{a} + q\vec{b} + q\vec{b} + r\vec{c} = p\vec{a} + 2q\vec{b} + r\vec{c}$ which produces a point at the center of the third face, and by translation, all 6 faces.

Thus we may have a face-centered orthorhombic lattice, F.

Case 3. Suppose p,q, and $r \neq 0$

$\vec{d} = p\vec{a} + q\vec{b} + r\vec{c} \in L$ but $\notin P$

A. $\rho\vec{d} = -p\vec{a} - q\vec{b} + r\vec{c}$ and $\vec{d} + \rho\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} - \rho\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

and we get the same results with the rotations σ and θ.

Note that $\rho\vec{d}$ produces a point in the center of an adjacent cell and likewise with σ and θ.

$\therefore$ We have found the body-centered orthorhombic lattice, I.

B. $m\vec{d} = p\vec{a} + q\vec{b} - r\vec{c}$ and $\vec{d} - m\vec{d} = 2r\vec{c} \Rightarrow r = 1/2$

$\vec{d} + m\vec{d} = 2p\vec{a} + 2q\vec{b} \Rightarrow p = 1/2$ and $q = 1/2$

$\therefore$ Again we will have the body-centered lattice, I.

Therefore in the Orthorhombic system we may have the primitive lattice, P, the end-centered lattice, A,B, or C, the face-centered lattice, F, or the body-centered lattice, I.

CASE VI. G contains no 3- or 4-fold axes, but there exists a unique axis (2-fold rotation, ρ, or a reflection, m)

We will form the primitive monoclinic lattice of the Monoclinic System.

Select $\vec{c}$ parallel to the axis, the shortest in that direction.

1. Suppose $\forall\ \vec{d} \in L$, $\vec{d} = k\vec{c} + \vec{d}'$ where $\vec{d}' \perp \vec{c}$ and $k \in Z$

   Select $\vec{a} \perp 1$, the shortest in its direction.

   Let $\vec{b} \perp 1$, $\vec{b} \nparallel \vec{a}$, the shortest in its derection

   Thus $a \neq b \neq c$ and $\alpha = \beta = 90 \neq \gamma$ determine the primitive monoclinic lattice shown in Figure 2-7.

   If $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c} \in L$ with $0 \leq p,q,r < 1$

   we may assume $r = 0$

   $\therefore\ \vec{d} = p\vec{a} + q\vec{b} \in L$

   Then $p = q = 0$ since every point in the parallelegram determined by $\vec{a}$ and $\vec{b}$ is closer to some vertex then $\vec{b}$, which contradicts our choice of $\vec{b}$.

   Thus there is no centering for this lattice.

2. Suppose $\exists\ \vec{d} \in L$, $\vec{d} = k\vec{c} + \vec{d}'$ where $\vec{d}' \perp \vec{c}$ and $k \notin Z$.

   $\vec{d} - m\vec{d} = 2r\vec{c}$ or $\vec{d} + \rho\vec{d} = 2r\vec{c}$

   $\therefore\ 2r \in Z$ and since $0 < r < 1$, we may assume $r = 1/2$

   Select $\vec{d} \ni \vec{d} = \frac{\vec{c}}{2} + \vec{d}'$ when $\vec{d}'$ is minimal

   Choose $\vec{a} = 2\vec{d}' = 2\vec{d} - \vec{c}$, which implies $\vec{a} \perp \vec{c}$ and it is the shortest vector in its direction.

   Let $\vec{b}$ be the shortest vector $\perp \vec{c}$, not $\parallel$ to $\vec{a}$.

We have now formed the same primitive monoclinic lattice, P, as in Figure 2-7.

Checking for centering in the second situations

Suppose $\vec{d} = p\vec{a} + q\vec{b} + \vec{c}/2 \in L$

1. We know that $\frac{\vec{a} + \vec{c}}{2} \in L$ by our choices of vectors.

   Thus $\exists$ an end-centered lattice, B, when $\vec{c}$ is the unique axis.

2. If $p = 0$, $\vec{d} = q\vec{b} + \frac{\vec{c}}{2}$

   $\vec{d} - m\vec{d} = 2q\vec{b} \Rightarrow q = 1/2$ where the plane of reflection m is normal to $\vec{b}$

   or $\vec{d} + \rho\vec{d} = 2q\vec{b} \Rightarrow q = 1/2$

   Thus $\exists$ an end-centered lattice, C, when $\vec{b}$ is the unique axis.

3. If neither p nor q equal zero, $\vec{d} = p\vec{a} + q\vec{b} + \frac{\vec{c}}{2}$

   $\rho\vec{d} = -p\vec{a} - q\vec{b} + \frac{\vec{c}}{2}$ hence $\vec{d} - \rho\vec{d} = 2p\vec{a} + 2q\vec{b}$

   and, $p = 1/2$ and $q = 1/2$

   $\therefore$ We have a point at the center of the cell.

   But then we may choose the lattice as in 1. and hence $\vec{d} = \frac{\vec{a} + \vec{c}}{2}$ and the lattice is end-centered. This change is shown in Figure 2.7.

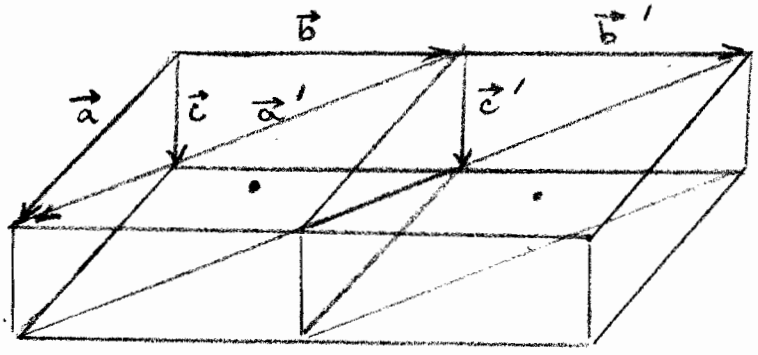


Figure 2-7

The vectors $\vec{a}'$, $\vec{b}'$, and $\vec{c}'$ represent situation 2. in forming the lattice.

Thus ∃ the primitive lattice, P, and the end-centered lattice, B or C in the Monoclinic System.

CASE VII. G contains no rotations of order 2,3, or 4 and there are no axes.

Choose $\vec{a}$ to be the shortest vector in one direction, $\vec{b}$, the shortest not parallel to $\vec{a}$, and $\vec{c}$, the shortest not parallel to the plane through $\vec{a}$ & $\vec{b}$. This forms the primitive triclinic lattice of the triclinic system.

In checking for centering suppose $\vec{d} = x\vec{a} + y\vec{b} + z\vec{c}$, where x,y, and z are not necessarily integers.

1. $y = z = 0$

   Then $x = n + r$ where $n \in Z$, $0 \leq r < 1$

   $\therefore\ \vec{d} - n\vec{a} = r\vec{a}$

   $|r\vec{a}| < |\vec{a}|$ and $\therefore\ r\vec{a} = 0 \Rightarrow r = 0$

2. $z = 0$

   Then $|\vec{d} - n\vec{a} - m\vec{b}| \leq |\frac{\vec{a} + \vec{b}}{2}| < |\frac{\vec{a}}{2}| + |\frac{\vec{b}}{2}| \leq |\vec{b}|$

   which is impossible.

3. $|\vec{d} - n\vec{a} - m\vec{b} - l\vec{c}| \leq \frac{(|\vec{a}|^2 + |\vec{b}|^2 + |\vec{c}|^2)^{1/2}}{2}$

   $\leq \frac{(3|\vec{c}|^2)^{1/2}}{2} < \frac{3^{1/2}}{2}|\vec{c}|$ which is again impossible since $\frac{3^{1/2}}{2} = \frac{1.732}{2} < 1$ and our choice of shortest vectors would be invalid.

Thus there is no centering in this system.

Chapter III

Point Groups, Holohedry, and Laue Groups

Now that we have found the fourteen Bravais lattices we can easily construct all the possible point groups for each lattice. As was mentioned in Chapter I, a point group is a group of symmetry operations which leave a point X and some 3-dimensional lattice containing X fixed. We will find the point groups for just one of the systems, the Tetragonal system, since a thorough coverage of all the systems is very lengthy and repetitious. The notation used by the International Tables for X-ray Crystallography will also be explained below and used in this work because we will need it to be able to continue our study.

Notation

1,2,3,4,6 represent x-fold rotations in the given axis.

$\bar{1},\bar{2},\bar{3},\bar{4},\bar{6}$ represent x-fold rotatory inversions in the given axis.

m symbolizes a reflection in the plane perpendicular to the given axis.

Section 1. - Point Groups

To begin forming the point groups we choose the axes from a certain lattice and find all the symmetries in each of these axes as we have done in the following example of the

tetragonal system:

Recall that the tetragonal system contains a 4-fold axis of rotation and we may have the primitive lattice P, or the body-centered lattice, I. Therefore we will consider the following five axes:

$$\vec{c},\ \vec{a},\ \vec{b},\ \overrightarrow{a+b},\ \overrightarrow{a-b}$$

We will initially use the symbols in Figure 3-1 to represent the elements of the point group by their action on the faces of a unit cell of the lattice which is centered at the fixed point X.

Temporary notation using the axes listed above

Symmetry elements

1 = identity

$\bar{1}$ = $(AA')(BB')(CC')$

$4\_\_\_\_$ = $(ABA'B')$

$(4\_\_\_\_)^2 = 2\_\_\_\_$ = $(AA')(BB')$

$(4\_\_\_\_)^3 = (4\_\_\_\_)^{-1}$ = $(AB'A'B)$

$\_2\_\_\_$ = $(BB')(CC')$

$\_\_2\_\_$ = $(AA')(CC')$

$m\_\_\_\_$ = (CC')

$\_m\_\_\_$ = (AA')

$\_\_m\_\_$ = (BB')

$\bar{4}\_\_\_\_$ = $(AB'A'B)(CC')$

$(\bar{4}\_\_\_\_)^{-1}$ = $(ABA'B')(CC')$

$\_\_\_\_m$ = $(AB')(A'B)$

$\_\_\_m\_$ = $(AB)(A'B')$

$\_\_\_\_2$ = $(AB')(A'B)(CC')$

$\_\_\_2\_$ = $(AB)(A'B')(CC')$

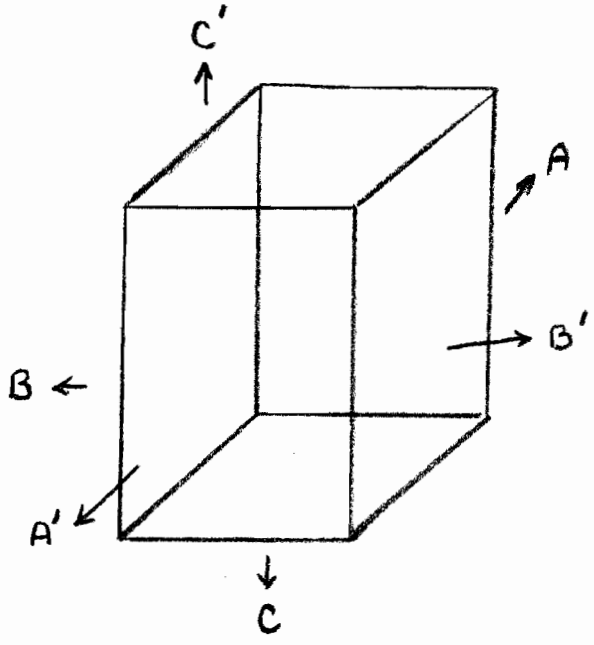


Figure 3-1

Now we must find all the subgroups of these elements, and in addition we will combine our five axes to form three types as is shown below. This is the method used in other Crystallographic work and is very useful to understand.

Subgroups

Axes: $\vec{c}$, $\vec{a}$, $\vec{b}$, $\overrightarrow{a+b}$, $\overrightarrow{a-b}$

Subgroup	Number of distinct subgroups of this type	Order
1	1	1
$\bar{1}$	1	2
2 1 1	1	2
1 2 1	2	2
1 1 2	2	2
m 1 1	1	2
1 m 1	2	2
1 1 m	2	2
4 1 1	1	4
$\bar{4}$ 1 1	1	4
2/m 1 1	5	4
2 2 1 or 2 1 2	2	4
2 m 1, 2 1 m, m 2 1 or m 1 2	4	4
$\bar{4}$ 2 m or $\bar{4}$ m 2	2	8
4 2 2	1	8
m m 1	2	8
4 m m	1	8
4/m 1 1	1	8
4/m m m	1	16

Note: When we use the notation X/m, this implies that both the rotation and reflection are associated with the same axis.

Finally we choose the subgroups in this list which do not occur in any of the simpler systems, and we have our list of point groups for the Tetragonal system:

4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$, $4/mmm$

Similar work may be done to obtain a complete list of point groups for all the systems, this list can be found in Table 3.1.

General Symbol	Triclinic	Monoclinic (1st setting)	Tetragonal	Trigonal	Hexagonal	Cubic
X	1	2	4	3	6	23
$\bar{X}$ (of even order)	–	$\bar{2}$ (≡m)	$\bar{4}$	–	$\bar{6}$	–
X plus center (includes $\bar{X}$ of odd order)	$\bar{1}$	2/m	4/m	$\bar{3}$	6/m	$2/m\,\bar{3}$ (m3)
	Monoclinic (2nd setting)	Orthorhombic				
X2	2 (≡1m)	222	422	32	622	432
Xm	m (≡1m)	mm2 (mm)	4mm	3m	6mm	–
$\bar{X}2$ or $\bar{X}m$ (of even order)	–	–	$\bar{4}2m$	–	$\bar{6}m2$	$\bar{4}3m$
X2 plus center Xm plus center (includes $\bar{X}m$ of odd order)	2/m	2/m 2/m 2/m (mmm)	4/m 2/m 2/m (4/mmm)	$\bar{3}$ 2/m ($\bar{3}$m)	6/m 2/m 2/m (6/mmm)	4/m $\bar{3}$ 2/m (m3m)

Section 2. - Holohedey

Another useful concept in Crystallography relates all the point groups which leave a particular lattice fixed. We know that any point group leaves a lattice fixed, so if we find all the point symmetries that leave this lattice fixed we have found what is called the holohedry of that lattice group. This classification is very useful in that it shows that there are only seven systems possible as well as making it easy to break down each holohedry and find that there are only 32 point groups.

The mathematical definition of holohedry is as follows:

Definition: The holohedry of a 3-dimensional lattice group L, at the point X is the group of all isometries, h, such that $h(x) = x$ and $h^i(L) = L$, i.e. the inner automorphism (h^i) leaves the lattice invariant.

Another definition would be, the largest crystallographic point group leaving X and the L-orbit of X invariant.

Again we will compute only one case since the work is tedious, but Table 3.2 lists all the holohedries. Since we have already worked with the tetragonal system we will do so again to make the work clearer.

Example:

Consider the primitive tetragonal lattice P. We have listed all the symmetry elements in Section 1 when finding the point groups. We then found all the subgroups and then

the point groups for that system. If you will review the work that was done there you can clearly see that all of the symmetry elements are contained in the point group 4/mmm. This is the largest point group which leaves the lattice fixed, and thus it is the holohedry.

Note that we will also have the same holohedry for the body-centered tetragonal lattice since the symmetry elements are the same as for the primitive lattice.

Therefore we can expect and do find one holohedry for each system, or likewise 7 systems for the 7 holohedries as listed in Table 3.2.

Table 3.2

System	Holohedry
Triclinic	$\bar{1}$
Monoclinic	2/m
Orthorhombic	mmm
Tetragonal	4/mmm
Cubic	m3m
Trigonal	$\bar{3}$m
Hexagonal	6/mmm

Section 3. - Laue Groups

In applying our knowledge of Crystallography, especially to use in X-ray diffraction, there is another important classification. This classification into what are called Laue groups deals with the groups that are obtained by adding a center of symmetry to the point groups. There are 11 centrosymmetrical point groups, and therefore 11 Laue groups, that is, classes of point groups which become identical when a center of symmetry is added to those that lack it. The point group of highest symmetry in each Laue group is the centrosymmetrical point group, and the symbol of this is used for the Laue group.

Before developing the Laue groups a brief description of their necessity and use is helpful. When working with X-ray diffraction as long as the wave-crystal interaction is not in the neighborhood of a resonance level, the intensity of X-ray reflection from a crystal without a center of symmetry is the same as one with this symmetry. That is, all coherent diffraction effects appear to be centrosymmetrical, even from non-centrosymmetrical crystals. Therefore the diffraction effects from a crystal of any class is that of the point group symmetry which is obtained by adding a center of symmetry to their actual symmetry elements where these are themselves non-centrosymmetrical. Thus there is reason for this further classification into Laue groups.

In forming the Laue groups we need simply to look at the point groups of a particular system. Take the Tetragonal system again. We have the point groups 4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}$2m, and 4/mmm.

1. Consider 4. By adding a center of symmetry we get an inversion in the center and a reflection with its plane normal to the axis of rotation. This yields 4/m.
2. Consider $\bar{4}$. Likewise we add m, yielding 4/m.
3. 4/m already contains a center of symmetry, thus it must be the symbol for a Laue group. This group contains 4, $\bar{4}$, and 4/m.
4. Consider 422. A canter of symmetry produces reflections in each of the three types of axes plus the inversion in the center, and we would now symbolize the group by 4/mmm.
5. & 6. 4mm and $\bar{4}$2m also do not have a center of symmetry, but when added yield 4/mmm.
7. 4/mmm contains a center of symmetry, thus is the symbol for another Laue group containing 422, 4mm, $\bar{4}$2m, and 4/mmm.

Now we have found two Laue groups and similar work in the other 6 systems will produce the 11 Laue groups as shown in Table 3.3.

Triclinic	Monoclinic	Tetragonal	Trigonal	Hexagonal	Cubic
1 $\bar{1}$	2 m $2/m$	4 $\bar{4}$ $4/m$	3 $\bar{3}$	6 $\bar{6}$ $6/m$	23 $m3$

Note: The symbol of the Laue group is that of the last point group in each rectangle.

Orthorhombic				
222 $mm2$ mmm	422 $4mm$ $\bar{4}2m$ $4/mmm$	32 $3m$ $\bar{3}m$	622 $6mm$ $\bar{6}m2$ $6/mmm$	432 $\bar{4}3m$ $m3m$

The 11 Laue Groups

Table 3.3

Chapter IV

Space Groups

We have now found all of the Bravais lattices and all the point groups. Recall that the lattices contain only the translations, and the point groups contain the rest of the symmetry elements without the translations. Our last classification will be into space groups from which both of the above were derived. Thus we have a group that contains all the symmetries of a crystal structure. The space group is actually the smallest group of symmetries of space which contains the whole lattice group and also the specific symmetries which we will name.

Remember that we mentioned that the combination of translations with some of the other symmetry elements yield new symmetry elements, these being the screw displacement (a rotation followed by a translation parallel to the axis of rotation), and the glide reflection (a reflection followed by a translation parallel to the plane of reflection). Thus every element of a space group can be factored as $\sigma \cdot \Gamma$, where σ is a rotation, a rotatory inversion, or a reflection, and Γ is a translation.

We will not go through all the cases to develope the 230 space groups, but a list of them is provided in Table 4-1. We will do several relavant examples that will show the procedure for several different situations, and the reader should refer to the International Tables for X-ray Crystallography for further help.

Example 1. Consider the Tetragonal system, in particular the point group 4, generated by a rotation ρ. Recall that the primitive tetragonal lattice is generated by $\vec{c}$, the shortest vector parallel to the axis of rotation, $\vec{a}$ is the shortest vector perpendicular to $\vec{c}$, and $\vec{b} = \rho(\vec{a})$.
The Bravais lattices of the Tetragonal system are the primitive lattice, P, and the body-centered lattice, I, both of which we must consider in forming the space groups.

Point group - 4

I. Lattice - P

Consider the kinds of 3-dimensional symmetries that have ρ as the non-translational aspect.

Let Γ be the translation determined by $\vec{c}/4$, and let L be the group of translations of P.

(a.) $P4_1$ is the symbol for the space group generated by L and $\rho\Gamma$.

Figure 4-1 demonstrates the action of $\rho\Gamma$ on points in this group.

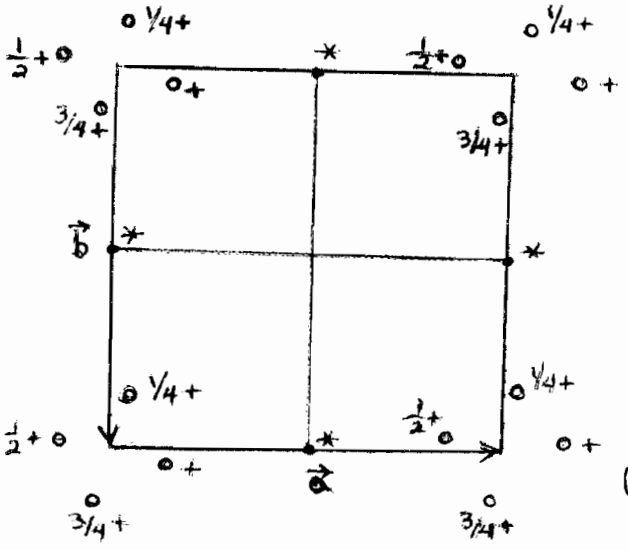


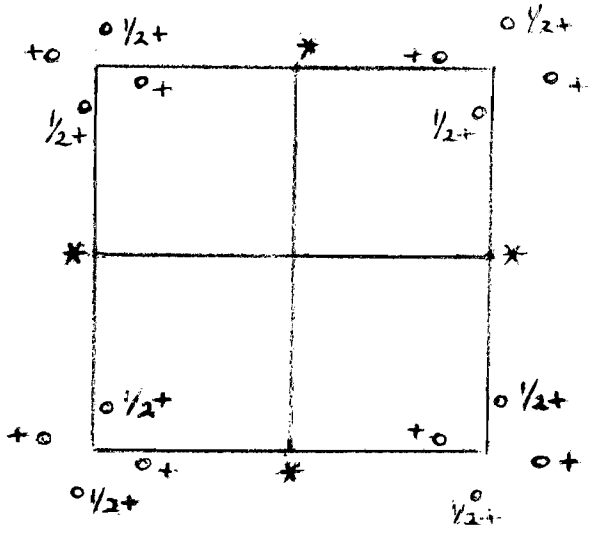
Figure 4-1

Note that $\rho\Gamma$ also induces a screw displacement of type 2_1 with axis $\|$ to $\vec{c}$ through the starred points. (*)

($\vec{c}$ is normal to the paper)

(b.) $P4_2$ is the symbol for the space group generated by L and $\rho\Gamma^2$.

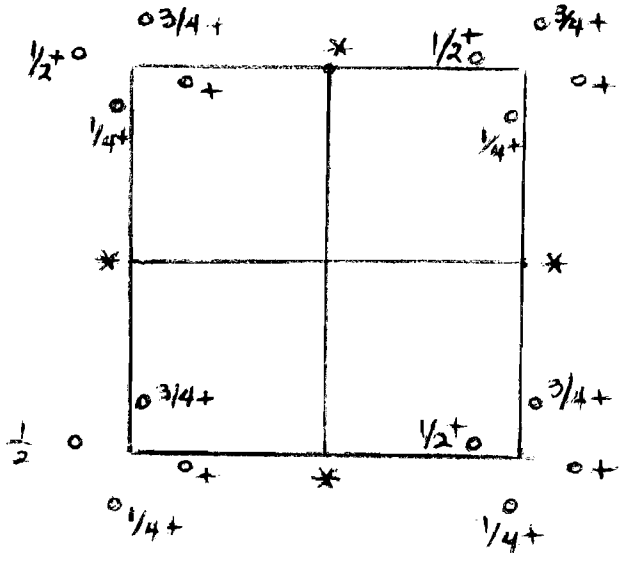
Figure 4-2 shows this group.



A rotation of the type 2 is also induced by $\rho\Gamma^2$, with axis || to c through the starred points.

Figure 4-2

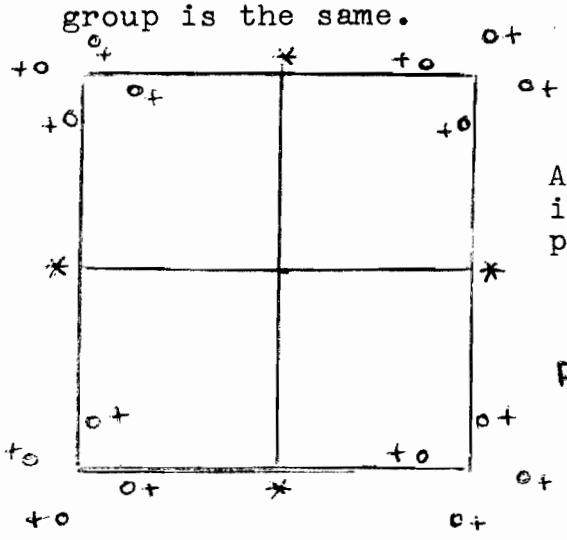
(c.) $P4_3$ is the symbol for the space group generated by L and $\rho\Gamma^3$ and shown in Figure 4-3.



Once again a screw displacement of the type 2, is produced as in (a.) at the starred points.

Figure 4-3

(d.) P4 is the space group generated by L and ρ. Since $\Gamma^4 \in L$, $\langle L, \rho\Gamma^4 \rangle = \langle L, \rho \rangle$, thus the space group is the same.



A rotation of type 2 is induced at the starred points.

Figure 4-4

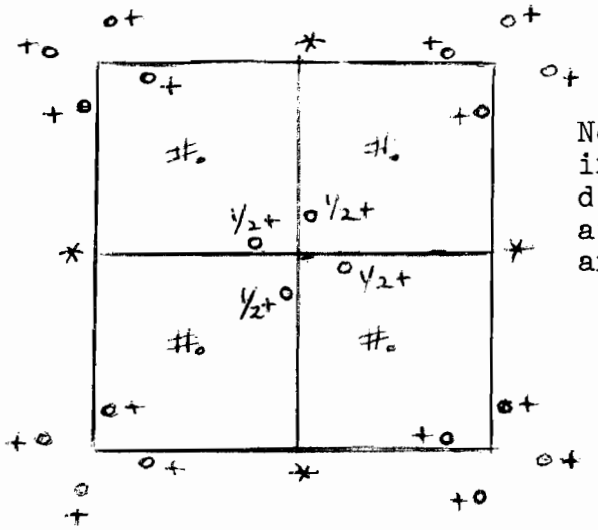
We have now considered all the possibilities with P.

II. Lattice - I

Recall that the lattice I now includes the vector $\vec{d} = \frac{\vec{a} + \vec{b} + \vec{c}}{2}$ as well as all vectors of P.

Let Γ be the translation determined by $\vec{c}/4$, and L, the group of translations of I.

(a.) I4 is the symbol for the space group generated by L and ρ as below.

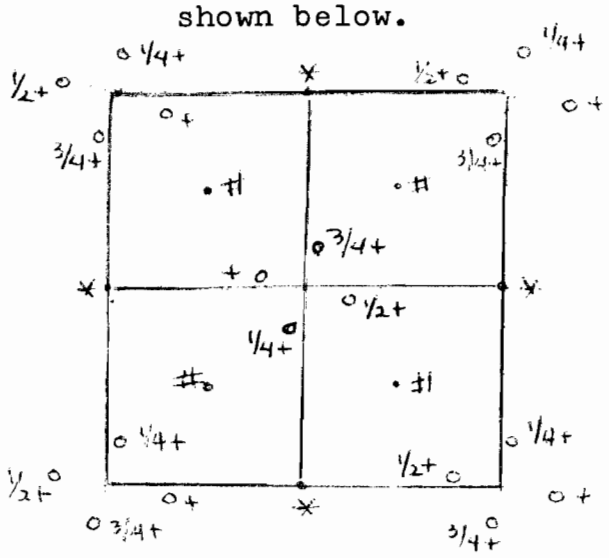


Note that in this group ρ induces two types of screw displacements, one type 4_2 at the starred points, (*), and type 2_1 at the points #.

Figure 4-5

Since we have seen the screw displacement of type 4_2 is also in I4, it is easy to realize that this group is essentially the same as the group generated by L and $\rho\Gamma^2$. If σ is the translation associated with $\vec{d}$, then $\rho\sigma$ and L generate the screw displacement of type 4_2.

(b.) $I4_1$ is the space group generated by L and $\rho\Gamma$ as shown below.



$\rho\Gamma$ also induces two types of screw displacements, type 4_3 at the points *, and simply 2 at the points #.

Figure 4-6

This group is essentially the same as the group generated by L and $\rho\Gamma^3$ since we have a screw displacement 4_3 that is generated by L and $\rho\sigma$, where σ is the translation associated with $\vec{d}$.

Thus there are 6 space groups formed from the point group 4 in the Tetragonal System.

Example 2. Consider the Monoclinic system, in particular the point group, m, generated by the reflection . Recall that the primitive monoclinic lattice is generated by vectors $\vec{a}, \vec{b}$, and $\vec{c}$ such that $a \neq b \neq c$ and $\alpha = \beta = 90 \neq$ as shown in Chapter II.

The Bravais lattices of the Monoclinic system are the primitive lattice, P, and the end-centered lattice, B (or C, by our choice of axis of rotation).

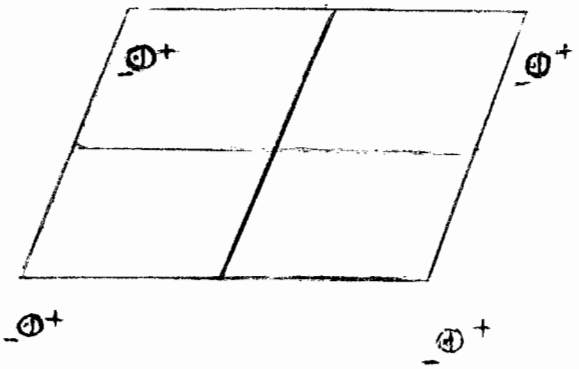
Point group - m

I. Lattice - P

Consider the kinds of 3-dimentional symmetries that have m as the non-translational aspect.

Let Γ be the translation determined by $\vec{c}/2$, and let L be the group of translations of P.

(a.) Pm is the symbol for the space group generated by L and m, as shown below.



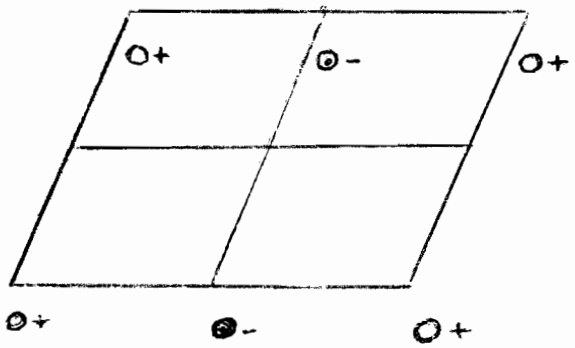
The reflection plane is parallel to the plane of projection.

Figure 4-7

Note: The symbol $\pm$ denotes two points, one above the plane and one below it.

(b.) Pb is the space group generated by L and

m_Γ = b, a glide reflection.



The glide plane is parallel to the plane of projection.

Figure 4-8

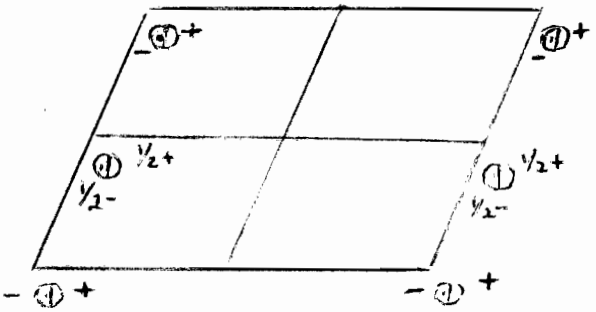
We have now considered all the possibilities with P.

II. Lattice - B

Recall that the lattice B now includes the vector $d = (\vec{a} + \vec{c})/2$ as well as all vectors of P.

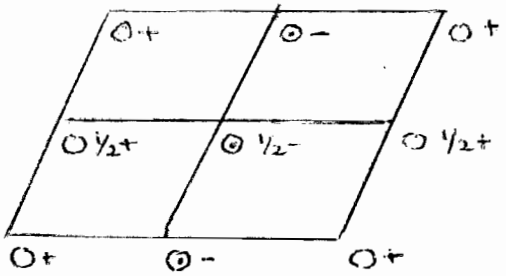
Γ will be the translation determined by $\vec{c}/2$, and L, the group of translations of B.

(a.) Bm is the space group generated by L and m.



The reflection plane is parallel to the plane of projection.

(b.) Bb is the space group generated by L and $m\Gamma$ = b.



The glide plane is parallel to the plane of projection.

Thus we have found all of the space groups that can be formed from the point group m.

Table 4.1

System	Holehedry	Laue group	Point group	Lattice	Space group
Triclinic	$\bar{1}$	$\bar{1}$	1	P	P1
			$\bar{1}$		P$\bar{1}$
Monoclinic	2/m	2/m	2	P	P2
					$P2_1$
				B or C	B2 or C2
			m	P	Pm
					Pb or Pc
				B or C	Bm or Cm
					Bb or Cc
			2/m	P	P2 or m
					$P2_1$ or m
				B or C	B2/m or C2/m
				P	P2/b or P2/c
					$P2_1/b$ or $P2_1/c$
				B or C	B2/b or C2/c
Orthorhombic	mmm	mmm	222	P	P222
					$P222_1$
					$P2_12_12$
					$P2_12_12_1$
				C	$C222_1$
					C222

System	Holehedry	Laue group	Point group	Lattice	Space group
Orthorhombic (cont.)				F	F222
				I	I222
					$I2_12_12_1$
			mm2	P	Pmm2
					$Pmc2_1$
					Pcc2
					Pma2
					$Pca2_1$
					Pnc2
					$Pmn2_1$
					Pba2
					$Pna2_1$
					Pnn2
				C	Cmm2
					$Cmc2_1$
					Ccc2
				A	Amm2
					Abm2
					Ama2
					Aba2
				F	Fmm2
					Fdd2
				I	Imm2
					Iba2
					Ima2

System	Holehedry	Laue group	Point group	Lattice	Space group
Orthorhombic (cont.)			mmm	P	Pmmm
					Pnnn
					Pccm
					Pban
					Pmma
					Pnna
					Pmna
					Pcca
					Pbam
					Pccn
					Pbcm
					Pnnm
					Pmmn
					Pbcn
					Pbca
					Pnma
				C	Cmcm
					Cmca
					Cmmm
					Cccm
					Cmma
					Ccca
				F	Fmmm
					Fddd
				I	Immm

System	Holdhedry	Laue group	Point group	Lattice	Space group
					Ibam
					Ibca
					Imma
Tetragonal	4/mmm	4/m	4	P	P4
		4/mmm			$P4_1$
					$P4_2$
					$P4_3$
				I	I4
					$I4_1$
			$\bar{4}$	P	$P\bar{4}$
				I	$I\bar{4}$
			4/m	P	P4/m
					$P4_2/m$
					P4/n
					$P4_2/n$
				I	I4/m
					$I4_1/a$
			422	P	P422
					$P42_12$
					$P4_122$
					$P4_12_12$
					$P4_222$
					$P4_22_12$
					$P4_322$

System	Holehedry	Laue group	Point group	Lattice	Space group
Tetragonal (cont.)					$P4_32_12$
				I	I422
					$I4_122$
			4mm	P	P4mm
					P4bm
					$P4_2cm$
					$P4_2nm$
					P4cc
					P4nc
					$P4_2mc$
					$P4_2bc$
				I	I4mm
					I4cm
					$I4_1md$
					$I4_1cd$
			$\bar{4}2m$	P	$P\bar{4}2m$
					$P\bar{4}2c$
					$P\bar{4}2_1m$
					$P\bar{4}2_1c$
					$P\bar{4}m2$
					$P\bar{4}c2$
					$P\bar{4}b2$
					$P\bar{4}n2$
				I	$I\bar{4}m2$
					$I\bar{4}c2$

System	Holehedry	Laue group	Point group	Lattice	Space group
					$I\bar{4}2m$
					$I\bar{4}2d$
			4/mmm	P	P4/mmm
					P4/mcc
					P4/nbm
					P4/nnc
					P4/mbm
					P4/mnc
					P4/nmm
					P4/ncc
					$P4_2/mmc$
					$P4_2/mcm$
					$P4_2/nbc$
					$P4_2/nnm$
					$P4_2/mbc$
					$P4_2/mnm$
					$P4_2/nmc$
					$P4_2/ncm$
				I	I4/mmm
					I4/mcm
					$I4_1/amd$
					$I4_1/acd$

System	Holehedry	Laue group	Point group	Lattice	Space group
Trigonal	$\bar{3}m$	$\bar{3}$	3	P	P3
		$\bar{3}m$			$P3_1$
					$P3_2$
				R	R3
					$P\bar{3}$
			$\bar{3}$	R	$R\bar{3}$
			32	P	P312
					P321
					$P3_112$
					$P3_121$
					$P3_212$
					$P3_221$
				R	R32
			3m	P	P3m1
					P31m
					P3c1
					P31c
				R	R3m
					R3c
			$\bar{3}m$	P	$P\bar{3}1m$
					$P\bar{3}1c$
					$P\bar{3}m1$
					$P\bar{3}c1$
				R	$R\bar{3}m$
					$R\bar{3}c$

System	Holehedry	Laue group	Point group	Lattice	Space group
Hexagonal	6/mmm	6/m 6/mmm	6	P	P6
					$P6_1$
					$P6_2$
					$P6_4$
					$P6_3$
			$\bar{6}$	P	$P\bar{6}$
			6/m	P	P6/m
					$P6_3/m$
			622	P	P622
					$P6_122$
					$P6_322$
					$P6_222$
					$P6_422$
					$P6_322$
			6mm	P	P6mm
					P6cc
					$P6_3cm$
					$P6_3mc$
			$\bar{6}m2$	P	P6m2
					$P\bar{6}c2$
					$P\bar{6}2m$
					$P\bar{6}2c$
			6/mmm	P	P6/mmm
					P6/mcc
					$P6_3/mcm$
					$P6_3/mmc$

System	Holehedry	Laue group	Point group	Lattice	Space group
Cubic	m3m	m3 m3m	23	P	P23
				F	F23
				I	I23
				P	$P2_13$
				I	$I2_13$
			m3	P	Pm3
					Pn3
				F	Fm3
					Fd3
				I	Im3
				P	Pa3
				I	Ia3
			432	P	P432
					$P4_232$
				F	F432
					4_132
				I	I432
				P	$P4_332$
					$P4_132$
				I	$I4_132$
			$\bar{4}3m$	P	$P\bar{4}3m$
				F	$F\bar{4}3m$
				I	$I\bar{4}3m$
				P	$P\bar{4}3n$
				F	$F\bar{4}3c$

System	Holehedry	Laue group	Point group	Lattice	Space group
Cubic (cont.)				I	$I\bar{4}3d$
			m3m	P	Pm3m
					Pn3n
					Pm3n
					Pn3m
				F	Fm3m
					Fm3c
					Fd3m
					Fd3c
				I	Im3m
					Ia3d

CONCLUSION

We have now classified all crystal structures into their basic groups, and have been able to show that these are the only types of structures that can be formed. From this point I hope that others will be able to proceed on with the study of crystallography in more detail, or to apply it to work in their respective fields.

Crystallography is a very broad and expanding field, the study of which has broadened my scope extensively into the applications and uses of my last four years of work in mathematics, for this I am very grateful. The preparatory work for the study was equally as useful as the findings in crystallography to me, in that I have had to combine the knowledge that I have obtained from various mathematics courses, and put it to use. I strongly recommend this study to all mathematics majors, and hope that they will find the work as interesting and useful as I have.