MAGNETIC SPACE GROUPS

by

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Laurea, Universita' di Palermo, 1957
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MAGNETIC SPACE GROUPS

ABSTRACT

Magnetic space groups (MSGs) were first introduced (under a different name) by Heesch more than 30 years ago, and a list of all of them was published by Belov, Neronova and Smirnova in 1955. However, no mathematically rigorous derivation of MSGs can be found in the existing literature, although an outline of a method for obtaining a large class of MSGs was published by Zamorzaev in 1957. In this thesis a systematic rigorous method for constructing MSGs is described in detail, and a proof that the method in fact gives all the MSGs is presented. The method also leads in a natural way to a new classification of MSGs which is useful for a systematic study of the arrangements of magnetic moments in ferromagnetic, ferrimagnetic and antiferromagnetic crystals.

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Magnetic space groups (MSGs) were first introduced (under a different name) by Heesch more than 30 years ago, and a list of all of them was published by Belov, Neronova and Smirnova in 1955. However, no mathematically rigorous derivation of MSGs can be found in the existing literature, although an outline of a method for obtaining a large class of MSGs was published by Zamorzaev in 1957. In this thesis a systematic rigorous method for constructing MSGs is described in detail, and a proof that the method in fact gives all the MSGs is presented. The method also leads in a natural way to a classification of MSGs which is useful for a systematic study of the arrangements of spins in ferromagnetic, ferrimagnetic and antiferromagnetic crystals. The first and the last chapter of the thesis deal with the physical aspects of the problem, the remaining chapters with purely mathematical aspects of it.
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CHAPTER 1

INTRODUCTION AND SUMMARY

This thesis is mainly devoted to a group theoretical derivation and classification of magnetic space groups (MSGs).

The reason for studying the MSGs is that they are groups of inhomogeneous linear space-time transformations which leave all possible three-dimensional periodical arrangements of magnetic moments invariant and hence are of importance for the theory of magnetically ordered crystals, that is, ferromagnetic, antiferromagnetic and ferrimagnetic crystals. By a "possible arrangement" of magnetic moments we mean an arrangement of magnetic moments which would certainly occur in nature if it had only to satisfy requirements of invariance under some of the space-time transformations just mentioned, but which may actually not occur if its existence violates some dynamical law. By "periodical" arrangement of magnetic moments we mean an arrangement of magnetic moments which has the translatory symmetry of a lattice.

The problem of deriving all MSGs is similar to that of deriving the groups which leave all possible three-dimensional periodical arrangements of atoms invariant. As is well known the solution to this problem is given by the theory of space groups. Obviously the two problems are not independent, since, in a magnetic crystal, individual magnetic moments are located at positions of magnetic atoms.
One is then naturally led to ask this question: how many different possible periodical arrangements of magnetic moments are there? The answer obviously depends on what one means by "different" arrangements of magnetic moments. If an arrangement of magnetic moments is invariant under a group of space-time transformations, and if a second arrangement of magnetic moments is invariant under a second group of space-time transformations, then the two arrangements will be called "different" if there exists no inhomogeneous space transformation which transforms one group into the other. According to this convention all the magnetic arrangements which are left invariant under groups transformable into one another by means of an inhomogeneous linear space transformation are not different. Thus to the arrangements of magnetic moments which are not different in our sense there corresponds a class of space-time transformation groups which can be transformed into one another by means of an inhomogeneous linear space transformation. The answer to the question formulated above is then that there are as many different possible periodical arrangements as there are classes of MSGs. If we refer to a class of MSGs as a MSG then we say that there are as many different possible arrangements of magnetic moments as there are MSGs.

In the course of this thesis we use the term MSG in both senses, that is, at times we use it to indicate a particular MSG, at other times we use it to indicate a class of MSGs. However, it should be clear from the context in which of the two senses the term is used.
Although what we have said about MSGs so far contains implicitly their definition, we have to state more precisely some properties of magnetically ordered crystals before we can formulate that definition explicitly.

As is well-known all magnetically ordered crystals can be divided into three classes (for simplicity, we consider here the case of zero temperature):

ferromagnetic crystals, where all the magnetic moments of the individual atoms are parallel and, hence, the macroscopic magnetic moment has the maximum value compatible with the magnitude of the individual magnetic moments;

antiferromagnetic crystals, where the macroscopic magnetic moment is zero, despite the fact that the individual magnetic moments are not oriented at random;

ferrimagnetic crystals, where the macroscopic magnetic moment is neither zero, nor has the maximum value compatible with the magnitude of the individual magnetic moments.

Obviously the crystals of the three classes have a common feature, a non-vanishing average magnetic moment of
individual magnetic atoms. This feature will suggest a natural definition of MSGs.

It is generally accepted that the Schroedinger equation of a perfect crystal considered as a system of nuclei and electrons is invariant under the operations of the direct product group $\tilde{F} \times \tilde{A}$, where $\tilde{F}$ is the space group of the crystal and $\tilde{A}$ is the time-reversal group consisting of the identity $E$ and the time-reversal operation $E'(t \rightarrow -t)$. (As we are interested only in the stationary states of the crystal, we disregard time-translations.)

(Strictly speaking the Schroedinger equation is not invariant under the group $\tilde{F} \times \tilde{A}$, but it is invariant under the group of state-vector transformations which correspond to the space-time transformations of $\tilde{F} \times \tilde{A}$. However as no quantum mechanical application of MSGs will be discussed in this thesis, and the quantum mechanical language will not be used except in the next few paragraphs, it would be exaggerated to introduce at this stage the concept of double magnetic space groups, analogous to that of double space groups.)

In the case of a magnetic crystal, in the absence of an external magnetic field, the Schroedinger equation is still invariant under the group $\tilde{F} \times \tilde{A}$ and hence in particular under time-reversal. However this time-reversal invariance is incompatible with the non-vanishing of the average magnetic moment of the individual atoms. In fact, if $\vec{m}$ is
the magnetic moment operator for an individual atom and $|\mu\rangle$ is an eigenstate of the system, the non-vanishing of the average individual magnetic moment implies that

$$\langle \vec{m} \rangle \equiv \text{Trace} \vec{m} \neq 0 \quad \text{where} \quad \text{Trace} \vec{m} = \sum_{\mu} \langle \mu | \vec{m} | \mu \rangle,$$

the sum being over all the eigenstates belonging to a given energy eigenvalue of the system. On the other hand the time-reversal invariance implies

$$\langle \vec{m} \rangle = \text{Trace} \vec{m} = 0$$

because both the eigenstate $|\mu\rangle$ and its time-reversed $|\mu\rangle_\theta$ are eigenstates belonging to the same energy eigenvalue of the system and $\vec{m}$ anticommutes with the time-reversal operator $\Theta$.

One has then to conclude that although the symmetry group of the Schroedinger equation of a magnetic crystal contains the time-reversal operator, an energy eigenstate and the corresponding time-reversed eigenstate cannot coexist if the crystal is magnetically ordered. In other words, the transition to the magnetically ordered state implies an apparent reduction of the symmetry of the problem: the physical properties of a magnetically ordered crystal are as if
the symmetry group of the Schroedinger equation was a subgroup of \( \tilde{F} \times \tilde{A} \)

(a) which does not contain the identity of \( \tilde{F} \) combined with time-reversal as an element,

and

(b) which is isomorphic to \( \tilde{F} \) or to a space group which is a subgroup of \( \tilde{F} \).

Each such subgroup \( \tilde{M} \) of \( \tilde{F} \times \tilde{A} \) is called magnetic space group. In general, we define an MSG as being any subgroup of \( \tilde{F} \times \tilde{A} \):

(a) which does not contain the identity of \( \tilde{F} \) combined with time-reversal as an element,

(b) which is isomorphic to some space group.

Since there is only one abstract group of order 2, the problem of constructing all MSGs is clearly independent of the physical meaning assigned to the element \( E' \) of the group \( \tilde{A} \). In fact, MSGs were first considered under a different name and in quite a different connection more than 30 years ago by Heesch (1930); he refers to them as "four-dimensional groups of the three-dimensional space". The analogous two-dimensional problem (that is the case in which \( \tilde{F} \) is a two-dimensional space group) has been considered and solved even earlier by Hermann (1928), Alexander and Herrman (1928), Weber (1929) and Heesch (1929). The motivation for introducing such new groups was at that time
either purely mathematical or crystallographical. The element E' of A was interpreted essentially as meaning the change of value of a coordinate capable of assuming two values, or as a change of colour in a plane ornament (assuming that exactly two colours were available). Of course, no reference to the problem of magnetic ordering was possible at this early stage of the history of the problem.

Heesch (1930) was not only the first to consider the MSGs in the sense just indicated, and to give a list of MSGs of the triclinic and monoclinic system, but also seems to have been the first to realize the importance of his groups from the physical point of view. He says "Hierdurch empfiehlt sich diese Koordinate (that is the coordinate mentioned above) als Vertreter einer jeden Eigenschaft des homogenen ebenen (but he has in mind also the three-dimensional case as is clear from the rest of his paper) Diskontinuums, die sich auf die Formel "plus-minus" bringen lasst, d.h. für jede "polare" Eigenschaft z.B. Besetzung mit zwei verschiedenen Ionen, Elektronenspin, elektrische Doppelschicht, magnetisches Blatt, Durchsetzung mit einer Dipolverteilung, reelles and virtuelles Bild, vorher-nachher, usw." Possibly the "vorher-nachher" could be interpreted as a reference to time-reversal, but no further mention of this possibility can be found in his paper.
Heesch also gave the complete list of what we will call the magnetic point groups (to be defined in Chapter 2), and he estimated the number of magnetic space groups to be close to 1800 (actually there are 1421 of them).

The complete list of MSGs has been published only in 1955 by Belov, Neronova and Smirnova (1955). These authors do not even mention Heesch's work, nor do they make any reference to the problem of magnetic ordering and to the importance of time-reversal in this connection. The same is true of Zamorzaev who has also given a list of MSGs in an unpublished thesis (1953) unavailable to us, and who published (1957) a short paper in which he outlines (without proofs) his method of deriving those MSGs which are isomorphic to the symmorphic space groups. What we call MSGs is called by Belov, Neronova and Smirnova, and by Zamorzaev, "Shubnikov groups", a name now widely used, not only in Russia, but hardly justified from the historical point of view.

A clear realization that MSGs are of importance for a systematic classification and discussion of magnetically ordered crystals, and that the element E' of $\tilde{A}$ must be interpreted in this connection as time-reversal, is due to Landau and Lifschitz. In fact the term "magnetic space groups" has been introduced by them.

The actual applications of the idea of Landau and Lifschitz to specific magnetic problems are very recent.

The first to apply MSGs to the problem of interpretation of magnetic neutron diffraction data were Donnay,
Corliss, Donnay, Elliott and Hastings (1958) and Le Corre (1958). Le Corre also discusses some other applications of MSGs.

As has been shown by Riedel and Spence (1960) and Van der Lugt (1961) nuclear magnetic resonance spectra in single crystals can also be interpreted in terms of MSGs.

Additional historical and bibliographical remarks will be found at the end of each chapter of this thesis (see also Donnay (1961)).

Although a list of all MSGs is available (Belov, Neronova and Smirnova, 1955, 1957) and some indications how to obtain it are given in the above-quoted papers by Heesch (1930), Belov, Neronova and Smirnova (1955) and Zamorzaev (1957), no rigorous and complete mathematical method of constructing all MSGs has been described in the existing literature. Such a method is described in this thesis, starting out from the definition of MSGs given above. (Strangely enough, not even this explicit definition can be found in the literature.) We present the method in such a way that its completeness is evident, in other words, we prove that there exists no MSG which is not obtainable by using our method.

In particular, in Chapter 2, we discuss some immediate consequences of our definition of MSG. We show that the problem of constructing all MSGs is easily reduced to the problem of finding all subgroups $\tilde{D}$ of index 2 of all
space groups $\tilde{F}$. This result is implicitly contained in Zamorzaev's paper (1957), and in a paper by Tavger and Zaitsev (1956) which deals with the similar but much easier problem of constructing all magnetic point groups).

In Chapter 3 we deduce rules for finding the $\tilde{D}'s$ of all symmorphic and non-symmorphic space groups, and we show that all the $\tilde{D}'s$ are in fact obtainable from our rules. In connection with the derivation of the rules it turns out to be useful to classify all the $\tilde{D}'$s into three different kinds.

Correspondingly in Chapter 4 we show that there are three different kinds of MSGs. In that chapter we also give the definition and the properties of the magnetic lattice and the magnetic point group belonging to an MSG. A complete list of magnetic lattices and magnetic point groups is given (which is not new). Finally we show that some MSGs are obtained more than once by means of our rules, and we indicate ways of dealing with this redundancy.

While in Chapters 2, 3 and 4 the physical meaning of the element $E'$ of $\tilde{A}$ does not play any role, in Chapter 5, where we briefly discuss magnetic moment arrangements in crystals, it becomes essential to interpret that element as time-reversal. In particular, we introduce in Chapter 5 the usual distinction between MSGs which may leave ferromagnetic crystals invariant and those which may not. We give an explanation based solely on symmetry, why ferromagnetic space
groups whose magnetic point groups contain elements of order higher than two cannot leave non-collinear ferrimagnetic crystals invariant. We also discuss the physical significance of the concept of a "family of MSGs" in connection with the identification of the MSG of a given arrangement of magnetic moments. Correspondingly, as an example of the classification of MSGs into families we list the MSGs of triclinic, monoclinic, trigonal, hexagonal and cubic systems arranged in that particular way (which is different from that used in the tables of Belov, Neronova and Smirnova (1957) at the end of the thesis.

The theory of MSGs is, of course, not exhausted by the contents of this thesis. An essential part of the theory is that which deals with the corepresentations (in the sense of Wigner) of the MSGs. The corepresentations of the MSGs have been discussed recently by Dimmock and Wheeler (1962a, 1962b). We have developed a more complete treatment of the corepresentations but it will not be included in this thesis.

Finally, we would like to mention that the MSGs as defined by us clearly do not leave invariant non-periodical arrangements of magnetic moments like the spiral arrangements,
which does not mean, however, that the MSGs are of no importance in this case.

Chapters 2, 3 and 4 form, except for minor changes, an essential part of a monograph "Magnetic Groups" to be published jointly with Prof. W. Opechowski who has supervised this work.
CHAPTER 2

SOME PROPERTIES OF MAGNETIC GROUPS AND THE IDEA OF A METHOD OF CONSTRUCTING THEM.

SECTION 2.1

In chapter 1 we have introduced the definition of a magnetic space group (MSG) which we repeat here for convenience in a somewhat different but equivalent form.

(2.1.1) A magnetic space group $\tilde{M}$ is any subgroup of any $\tilde{F} \times \tilde{A}$ which satisfies the two following conditions:

(a) it does not contain the element $E E'$,

(b) it is isomorphic to $\tilde{F}$.

Here $\tilde{F}$ is any space group (elements: $F_1 = E$ (identity), $F_2, F_3, \ldots$), $\tilde{A}$ is the group consisting of two elements $A_1 = E$ (identity), $A_2 = E'$ (time-reversal), and the elements of the direct product $\tilde{F} \times \tilde{A}$ are pairs $FA$, an element of $\tilde{F}$ being always written on the left and an element of $\tilde{A}$ on the right. However, as already mentioned in Chapter 1, we may regard the group $\tilde{A}$ as the abstract group of order 2 as long as we do not apply the arguments and results of this chapter to physics.

Since $\tilde{F}$ in definition (2.1.1) is an arbitrary space group, and each space group is a subgroup of the general inhomogeneous linear group $\tilde{G}$, definition (2.1.1) can be replaced by the following equivalent one:
(2.1.2) A magnetic space group \( \tilde{\mathcal{M}} \) is any subgroup of \( \tilde{G} \times \tilde{A} \) which satisfies conditions (a) and (b) stated in (2.1.1).

In particular, it follows from (2.1.1), or (2.1.2), that every space group is an MSG. We shall occasionally call MSGs which are not simply space groups "non-trivial" MSGs.

It is convenient to define magnetic rotation groups, and magnetic lattices in an analogous manner:

(2.1.3) Let \( \tilde{\mathcal{R}} \) be the group of all proper and improper rotations (in the three-dimensional Euclidean space); a magnetic rotation group \( \tilde{\mathcal{R}}_M \) is then any subgroup of \( \tilde{\mathcal{R}} \times \tilde{A} \) which does not contain the element \( EE' \).

(2.1.4) If a magnetic rotation group is isomorphic to any one of the crystallographic point groups it will be called a magnetic point group.

(2.1.5) Let \( \tilde{T} \) be a lattice (i.e. a group of primitive translations in the three-dimensional Euclidean space); a magnetic lattice \( \tilde{\mathcal{N}}_M \) is then any subgroup of \( \tilde{T} \times \tilde{A} \) which does not contain the element \( EE' \), and which contains three linearly independent translations.

It follows from these definitions that "ordinary" rotation groups and "ordinary" lattices are special cases of magnetic rotation groups and magnetic lattices.

We see from the above definitions that magnetic groups of all three varieties (i.e. magnetic space groups, magnetic rotation groups and magnetic lattices) are always
subgroups of a direct product group of the form $\tilde{G} \times \tilde{A}$, where $\tilde{G}$ is different in each of the three cases but $\tilde{A}$ is always the same group of two elements. That is why, in Section 2.2 we define a mathematical analogue of magnetic groups for the case that $\tilde{G}$ in $\tilde{G} \times \tilde{A}$ is arbitrary, and discuss some of the consequences of that more general definition.

In Section 2.3 we specialize the results of Section 2.2 to the case of magnetic groups.

**SECTION 2.2**

Let $\tilde{G} \times \tilde{A}$ be the direct product of an arbitrary group $\tilde{G}$, whose elements will be denoted by $G$, and the group $\tilde{A}$ of order 2, whose elements will be denoted by $A$, or, more specifically, by $E$ (the identity) and $E'$. The elements of this direct product are pairs $GA$, an element of $\tilde{G}$ being always written on the left and an element of $\tilde{A}$ on the right.

We shall call an element $GA$ of $\tilde{G} \times \tilde{A}$ "primed" if $A = E'$, and "unprimed" if $A = E$. In particular, we shall call the element $EE'$ the "primed identity".

We shall often use a simplified notation: $G$ for $GE$, and $G'$ for $GE'$.

From these definitions it follows immediately that:

(2.2.1) The product of any two unprimed elements is unprimed.

(2.2.2) The product of any two primed elements is unprimed.
(2.2.3) The product of a primed element with an unprimed one (in either order) is primed.

We now define for each given, arbitrary $\tilde{G}$ a class of groups which we shall call $m$-groups; the letter "$m$" in "$m$-groups" is supposed to indicate that, for an appropriate choice of $\tilde{G}$, $m$-groups become magnetic groups of one of the three kinds introduced in Section 2.1.

(2.2.4) An $m$-group of $\tilde{G} \times \tilde{A}$ (or belonging to $\tilde{G} \times \tilde{A}$) is any subgroup of $\tilde{G} \times \tilde{A}$ which does not contain the primed identity $EE'$.

Obviously, the $m$-groups are of two kinds: those which consist entirely of unprimed elements of $\tilde{G} \times \tilde{A}$, and those which contain some primed elements. The former will be called "trivial" $m$-groups, the latter "non-trivial" $m$-groups.

(2.2.5) By omitting the primes in the elements of an $m$-group one obtains a subgroup of $\tilde{G}$ which is isomorphic to the $m$-group.

This theorem follows immediately from the definition (2.2.4) of $m$-groups and (2.2.1), (2.2.2), 2.2.3).

(2.2.6) The unprimed elements of a non-trivial $m$-group constitute a subgroup of index 2.

The proof of (2.2.6) follows from the following theorem valid for any group $\tilde{K}$:

(2.2.7) A subgroup $\tilde{L}$ of a group $\tilde{K}$ is a subgroup of index 2 if and only if the product of two arbitrary elements
of $\tilde{K}$ not belonging to $\tilde{L}$ is an element belonging to $\tilde{L}$.

In fact, since, according to (2.2.1), the product of any two unprimed elements of an $m$-group is an unprimed element, the unprimed elements form a subgroup of it. That the subgroup is of index 2 follows immediately from (2.2.7) in conjunction with (2.2.2).

Theorems (2.2.5) and (2.2.6) taken together simply mean that every $m$-group is isomorphic to some subgroup $\tilde{H}$ of $\tilde{G}$ and that $\tilde{H}$ then necessarily has a subgroup of index 2. Hence, conversely, one will obtain all non-trivial $m$-groups of $\tilde{G} \times \tilde{A}$ if one applies the following rule:

(2.2.8) Find all those subgroups $\tilde{H}$ of $\tilde{G}$ which have subgroups $\tilde{D}^{H}$ of index 2. For each $\tilde{D}^{H}$ of each $\tilde{H}$ combine the elements of $\tilde{D}^{H}$ with the identity $E$ of $\tilde{A}$ and the elements of the coset $\tilde{H} - \tilde{D}^{H}$ with the element $E'$ of $\tilde{A}$. The set of all elements of $\tilde{D}^{HE}$ and $(\tilde{H} - \tilde{D}^{H})E'$ will then necessarily constitute an $m$-group of $\tilde{G} \times \tilde{A}$ (because the set is obviously a subgroup of $\tilde{G} \times \tilde{A}$, and does not contain the element $EE'$).

An $m$-group obtained in this way from a given $\tilde{H}$ and $\tilde{D}^{H}$ will be denoted by $\tilde{M}(\tilde{D}^{H})$.

SECTION 2.3

In this section we specialize the general results of Section 2.2 to the case of magnetic groups.

Take the group $\tilde{G}$ of Section 2.2 to be the general inhomogeneous linear group $\tilde{G}$. Then, in view of (2.2.5) and
of the fact that all space groups, all rotation groups and all lattices are subgroups of \( \mathfrak{G} \), the definitions, given in Section 2.1, of the three types of magnetic groups can be reformulated as follows:

\( (2.3.1) \) Magnetic space groups \( \tilde{M} \) are those m-groups of \( \mathfrak{G} \times \tilde{A} \) which are isomorphic to space groups \( \mathcal{F} \).

\( (2.3.2) \) Magnetic rotation groups \( \tilde{R}_M \) are those m-groups of \( \mathfrak{G} \times \tilde{A} \) which are isomorphic to rotation groups \( \mathcal{R} \).

\( (2.3.3) \) Magnetic lattices \( \tilde{T}_M \) are those m-groups of \( \mathfrak{G} \times \tilde{A} \) which are isomorphic to lattices \( \tilde{T} \).

The rule \( (2.2.8) \) can then be directly applied to the three cases. In the case of MSGs the subgroups \( \tilde{H} \) are the space groups, and these are known. The problem of finding all MSGs has thus been reduced to the problem of finding all subgroups \( \tilde{D}^F \) of index 2 of all space groups \( \mathcal{F} \).

\( (2.3.4) \) A space group \( \tilde{F} \) and the MSGs obtained by means of rule \( (2.2.8) \) from all the \( \tilde{D}^F \)'s of \( \mathcal{F} \) will be said to form the "family" of \( \mathcal{F} \).

As is well-known (see, for example, Lomont (1959)), two space groups are regarded as belonging to the same class of space groups and are denoted by the same crystallographic symbol if and only if they are conjugate subgroups of the general inhomogeneous linear group .

Similarly, two MSGs will be regarded as belonging to the same class of MSGs, and denoted by the same crystallographic symbol (the notation used will be explained in
Chapter 4) if and only if they are conjugate subgroups of the direct product group $\tilde{\mathcal{G}} \times \tilde{\mathcal{A}}$.

Two space groups which do not belong to the same class of space groups will be occasionally referred to as "properly different". Similarly, two MSGs which do not belong to the same class of MSGs will be occasionally referred to as "properly different".

Perhaps it should be mentioned in passing that $M(D_1^F)$ and $M(D_2^F)$ may very well be properly different even though $D_1^F$ and $D_2^F$ are not properly different. This point and similar questions will be discussed later on (Section 4.3).

In the following chapters we shall need a more explicit notation for the elements of a space group, and of an MSG. We shall denote, as is customary, an element of a space group $\tilde{\mathcal{F}}$ by $(R | \tau(R) + t)$ where $R$ is a proper or improper rotation, $\tau(R)$ the non-primitive translation (which is always zero for the symmorphic space groups) belonging to $R$, and $t$ a primitive translation. The elements of an MSG are then of the form $(R_i \tau(R_i) + t_i) \in$ and $(R_i \tau(R_i) + t_i)'$, where $(R_i \tau(R_i) + t_i)$ belongs to $D_F$, and $(R_i \tau(R_i) + t_i)$ belongs to the coset $\tilde{\mathcal{F}} - D_F$. In most cases the simplified notation, introduced at the beginning of Section 2.2, will be used: $(R_i \tau(R_i) + t_i)$ for an unprimed element of an MSG, and $(R_i \tau(R_i) + t_i)'$ for a primed element.
NOTES TO CHAPTER 2

The procedure summarized in theorem (2.2.8) is a straightforward generalization of the well-known procedure to find all subgroups of the group \( \tilde{\mathfrak{H}} \) of all proper and improper rotations which do not contain space inversion. (See, for example, Weyl (1952), Appendix B). The group \( \tilde{\mathfrak{H}} \) is a direct product \( \tilde{\mathfrak{H}}_{pr} \times \tilde{I} \) where \( \tilde{\mathfrak{H}}_{pr} \) is the group of all proper rotations and \( \tilde{I} \) is the group consisting of identity and space inversion.

Most of the theorems proved in this chapter can be found stated, in a less general form and without proofs, in Zamorzaev (1957). As has already been mentioned in Chapter 1, Zamorzaev speaks of Shubnikov groups rather than MSGs and regards his method of constructing Shubnikov groups as being "essentially the Shubnikov method" (Shubnikov, 1951). However, Shubnikov has not considered the three-dimensional case. Zamorzaev's theorem 3 says essentially the same as our definition (2.1.1) of MSG.

Zamorzaev's definition of Shubnikov groups is contained in the following two paragraphs (we quote from the English translation):

"We shall define a Fedorov group as a group of spatial symmetry transformations (which we shall call homologous) with the following properties:

1) there exists a sphere of sufficiently large radius \( R \) such that no matter where it is located in space there lie within it homologous images of any arbitrary previously given point of space (homogeneity) and

2) there is at least one point in the space which has no homologous images arbitrarily close to it (discreteness).
Let us now assign positive (+) or negative (−) signs to the points of space and define a Shubnikov group as a group of symmetry and antisymmetry transformations, which we shall call homologous and antihomologous, respectively, which fulfills the following requirements: property 1) (homogeneity) is now fulfilled by both homologous and antihomologous images of a point, and property 2) (discreteness is maintained in its previous form."

We give here a brief dictionary of terms as used by Zamorzaev and other Russian authors, and by ourselves.

The dictionary of terms is as follows:
\[ \tilde{A} = \text{time-reversal group} = \text{antisymmetry group} = \text{change-of-color group}, \]
\[ \tilde{M}(\neq \tilde{F}) = \text{non-trivial MSG} = \text{black and white space group} = \text{minor Shubnikov group}. \]
\[ \tilde{F} \times \tilde{A} = \text{grey space group} = \text{major Shubnikov group}. \]
\[ \tilde{F} = \text{ordinary space group} = \text{Fedorov group} = \text{colourless space group}. \]
CHAPTER 3

DERIVATION OF RULES FOR CONSTRUCTING ALL SUBGROUPS OF INDEX 2 OF ALL SPACE GROUPS.

In this chapter we describe a systematic and exhaustive method of constructing all the subgroups $D^F$ of index 2 of all space groups $F$. In our discussion of this problem we take the knowledge of the properties of space groups for granted. For the basic definitions and properties we refer the reader to Koster (1957) and Lomont (1959); a detailed description of all space groups is given in "International Tables for X-Ray Crystallography" (1952).

In Section 3.1 we systematically derive the necessary conditions for sets of elements of $F$ to be subgroups $D^F$; this enables us to formulate rules for constructing all such sets. In many cases the conditions are also sufficient, but not always. The sufficient conditions are derived in Section 3.2.

The rules of Section 3.1 and 3.2 require, for most space groups $F$, the knowledge of all subgroups $R^D$ of index 2 of their point groups, and of all subgroups $T^D$ of index 2 of their lattices. Section 3.3 is devoted to a survey of the subgroups $R^D$ and $T^D$.

In Section 3.4 examples are given of the construction of all $D^F$'s for a few $F$'s using the rules of Section 3.1 and 3.2, and the data of Section 3.3.

The following convention will often be used in denoting the
elements of the various groups considered in this chapter
(and in the following chapters):

Let $\wedge H$ be a group and $D^H$ one of its subgroups of
index 2. An element of $\wedge H$ which belongs to $D^H$ will be labeled
with a Latin subscript, e.g. $H_a$, $H_b$, $H_c$, etc. ("Latin
elements"); an element of $\wedge H$ which does not belong to $D^H$
(it belongs then to the coset $\wedge H - D^H$) will be labeled with
a Greek subscript, e.g. $H_\alpha$, $H_\beta$, $H_\gamma$ etc. ("Greek elements").

SECTION 3.1

Let $(R \mid \tau(R)+t)$ be the general element of a space
group $\wedge F$. The letter $R$ denotes a proper or improper rotation
of the point group $\wedge R$ belonging to $\wedge F$. The symbol $\tau(R)$
denotes a non-primitive translation belonging to $R$ of the form
$\tau(R) = \nu_1 \alpha_1 + \nu_2 \alpha_2 + \nu_3 \alpha_3$. Here $a_1, a_2, a_3$ are the three
basic primitive translations of the lattice $\wedge T$ of $\wedge F$, and
$\nu_1, \nu_2, \nu_3$ are numbers whose absolute values are smaller
than unity. Finally the letter $t$ denotes a primitive
translation of $\wedge T$.

Let $(R^X | \sigma(R^X)+t^X)$ be the general element of a sub-
group $D^F$ of index 2 of $\wedge F$. For simplicity, from now on, we
write $\wedge D$ instead of $D^F$, as no confusion can arise. Here $R^X$
denotes a proper or improper rotation of the point group $\wedge R^X$
belonging to $\wedge D$; $\sigma(R^X)$ denotes a non-primitive translation
corresponding to $R^X$ and $t^X$ denotes a primitive translation
of the lattice $T^X$ of $\wedge D$. 
Obviously $\tilde{R}^X$ and $\tilde{T}^X$ are (proper or improper) subgroups of $\tilde{R}$ and $\tilde{T}$ respectively.

If the point group $\tilde{R}^X$ is a proper subgroup of $\tilde{R}$ we shall denote the subgroup $\tilde{D}$ by $\tilde{D}_T$; if $\tilde{R}^X$ is the point group $\tilde{R}$ itself the subgroup $\tilde{D}$ will be denoted by $\tilde{D}_R$.

Subgroups $\tilde{D}_T$.

We first state two theorems concerning $\tilde{D}_T$:

(3.1.1) The lattice of $\tilde{D}_T$ is necessarily identical with the lattice $\tilde{T}$ of $\tilde{F}$.

(3.1.2) The point group of $\tilde{D}_T$ is necessarily a subgroup $\tilde{R}^D$ of index 2 of the point group $\tilde{R}$ of $\tilde{F}$.

Proof of (3.1.1) follows from the observation that if the lattice of $\tilde{D}_T$ were a proper subgroup of $\tilde{T}$ then $\tilde{D}_T$ would be a subgroup of $\tilde{F}$ of an index higher than 2.

To prove (3.1.2) consider any two elements of the coset $\tilde{F}-\tilde{D}_T$ of $\tilde{D}_T$, $(R_1 | \tau(R_1)+t_1)$ and $(R_2 | \tau(R_2)+t_2)$. Here $R_1$ and $R_2$ belong to $\tilde{R}-\tilde{R}^X$ and $t_1$ and $t_2$ belong to $\tilde{T}$. Since $\tilde{F}$ is a space group, its lattice $\tilde{T}$ is invariant under $\tilde{R}$, that is $R_1t_2 \in \tilde{T}$ for any choice of $R_1 \in \tilde{R}-\tilde{R}^X$ and $t_2 \in \tilde{T}$. Since $\tilde{D}_T$ is a subgroup of index 2 of $\tilde{F}$ according to theorem (2.2.7) the product $(R_1R_2 | \tau(R_1)+R_1 \tau(R_2)+t_1+R_1t_2)$ belongs to $\tilde{D}_T$. This is the case only if $R_1R_2 \in R^X$ or, using theorem (2.2.7) again, if $\tilde{R}^X = \tilde{R}^D$.

From (3.1.2) it follows:

(3.1.3) A space group $\tilde{F}$ has no subgroups of the type $\tilde{D}^T$ if its point group has no subgroups of index 2.
If the point group $\tilde{R}$ of $\tilde{F}$ has subgroups $\tilde{R}^D$ of index 2 then theorems (3.1.1) and (3.1.2) give immediately the following rule for constructing all subgroups $\tilde{D}_T$ of $\tilde{F}$:

(3.1.4) Take the set $\Gamma$ of all those elements $(R_a \mid \tau(R_a) + t)$ of $\tilde{F}$ for which $R_a$ belongs to some specified $\tilde{R}^D$ and $t$ is any translation of the lattice $\tilde{T}$ of $\tilde{F}$. The set obviously constitutes a $\tilde{D}_T$. By taking all the $\tilde{R}^D$'s in turn one obtains all the $\tilde{D}_T$'s of $\tilde{F}$.

Next we consider the question, under which conditions a subgroup $\tilde{D}_T$ will be symmorphic.

If $\tilde{F}$ is a symmorphic space group, then obviously every subgroup $\tilde{D}_T$ of it is a symmorphic space group too. Its general element is $(R_a \mid t)$ with $R_a$ belonging to a subgroup $\tilde{R}^D$ of $\tilde{R}$ and $t$ belonging to $\tilde{T}$.

In a non-symmorphic space group $\tilde{F}$ the elements with no non-primitive translations form obviously a subgroup of $\tilde{F}$. If the point group belonging to such a subgroup of $\tilde{F}$ is a subgroup of index 2 of the point group $\tilde{R}$ of $\tilde{F}$, then obviously the space group $\tilde{F}$ has a symmorphic subgroup $\tilde{D}_T$. Otherwise any subgroup $\tilde{D}_T$ of a non-symmorphic space group $\tilde{F}$ is a non-symmorphic space group too. Its general element is $(R_a \mid \tau(R_a) + t)$ where again $R_a \in \tilde{R}^D$, $t \in \tilde{T}$. It should be noticed that in this case $\sigma(R_a) = \tau(R_a)$.

Subgroups $\tilde{D}_R$.

The point group of $\tilde{D}_R$ is by definition identical with the point group of $\tilde{F}$; hence, obviously:
(3.1.5) The lattice $\tilde{T}^D$ of $\tilde{D}_R$ is a subgroup of index 2 of the lattice $\tilde{T}$ of $\tilde{F}$.

From (3.1.5) it does not follow, however, that translations which belong to $\tilde{T} - \tilde{T}^D$ cannot occur as translations in the elements of $\tilde{D}_R$. It only follows that if they do occur they must be non-primitive translations of $\tilde{D}_R$. Hence the subgroups $\tilde{D}_R$ may be of two kinds: those, denoted by $\tilde{D}_{Ro}$, in whose elements no translations of $\tilde{T} - \tilde{T}^D$ occur; and those, denoted by $\tilde{D}_{Ra}$, in whose elements the translations of $\tilde{T} - \tilde{T}^D$ do occur. Obviously, one can always choose as one of the three basic primitive translations of $\tilde{T}$ a translation belonging to $\tilde{T} - \tilde{T}^D$. Let the translation so chosen be $t_\alpha$. Since $\tilde{T}^D$ is a subgroup of index 2 of $\tilde{T}$, every translation of $\tilde{T}$ belonging to $\tilde{T} - \tilde{T}^D$ can be expressed as a sum of $t_\alpha$ and a translation belonging to $\tilde{T}^D$.

(3.1.6) An element of $\tilde{D}_R$ is of the form:

$$\begin{align*}
(R | \sigma(R) + t_\alpha) & \quad \text{where} \quad R \in \tilde{R}, \quad t_\alpha \in \tilde{T}^D, \\
\sigma(R) &= \begin{cases} 
\tau(R) & \text{if} \quad \tilde{D}_R = \tilde{D}_{Ro} \\
\tau(R) + t_\alpha(R) & \text{if} \quad \tilde{D}_R = \tilde{D}_{Ra} \end{cases}
\end{align*}$$

and

$t_\alpha(R)$ may be either zero or equal to $t_\alpha$; the latter possibility must occur for at least one element of $\tilde{R}$. (We assume...
here that by no choice of the coordinate system can \( t_a \) be transformed away from all the elements of \( \tilde{D}_{Ra} \); for if this was possible the group in question would not be \( \tilde{D}_{Ra} \) but \( \tilde{D}_R \).

Since \( \tilde{D}_R \) is a space group its lattice must be invariant under any rotation of its point group. Or, more precisely, for any \( R \) belonging to the point group \( \tilde{R} \) of \( \tilde{D} \) and any \( t_a \) belonging to the lattice \( \tilde{T}^D \) of \( \tilde{D}_R \), one must have

\[
(3.1.7) \quad R t_a = t_b
\]

where \( t_b \) belongs to \( \tilde{T}^D \). But the point group \( \tilde{R} \) of \( \tilde{D}_R \) is also the point group of that \( \tilde{F} \) of which \( \tilde{D}_R \) is a subgroup of index 2. Hence:

\[
(3.1.8) \quad \text{The lattice } \tilde{T}^D \text{ of } \tilde{D}_R \text{ and the lattice } \tilde{T} \text{ of } \tilde{F} \text{ have the same holohedry, the "holohedry" of a lattice being, according to the usual definition, the largest point group which leaves the lattice invariant. (Of course, the point group } \tilde{R} \text{ need not be the holohedry of the two lattices.)}
\]

**Subgroups \( \tilde{D}_{Ro} \).**

To construct all the subgroups \( \tilde{D}_{Ro} \) of a given space group \( \tilde{F} \) one has thus, in view of (3.1.6), the following rule:

\[
(3.1.9) \quad \text{Take the set } \Delta \text{ of all those elements (}R | t(R) + t_a) \text{ of } \tilde{F} \text{ for which } t_a \text{ belongs to some specified } \tilde{T}^D \text{ which has the same holohedry as } \tilde{T} \text{ and } R \text{ is any rotation of the point group } \tilde{R} \text{ of } \tilde{F}. \text{ If the set } \Delta \text{ forms a group then it will be necessarily a subgroup } \tilde{D}_{Ro}. \text{ By taking all such } \tilde{T}^D's \text{ in turn one obtains all the } \tilde{D}_{Ro}'s \text{ of } \tilde{F}. \text{ The conditions}
for the set $\Delta$ to form a group are discussed later on in Section 3.2. The list of all subgroups $\tilde{T}^D$ (there are at most 7 of them) of a given lattice $\tilde{T}$ is given in Section 3.3. It is obvious from (3.1.9) that $\tilde{D}_{\tilde{R}0}$ is or is not symmorphic, according as $\tilde{F}$ is or is not symmorphic.

Subgroups $\tilde{D}_{\tilde{R}a}$.

In order to formulate the rules for constructing all the $\tilde{D}_{\tilde{R}a}$'s of a given space group $\tilde{F}$, it is convenient to discuss several possible cases separately. We shall discuss the several possible cases (they obviously exhaust all possibilities) in the following order:

A) $\tilde{F}$ whose point group $\tilde{R}$ has subgroups $\tilde{R}^D$:

A1) symmorphic $\tilde{F}$;

A2) non-symmorphic $\tilde{F}$ whose point group $\tilde{R}$ does not contain elements of order higher than 2;

A3) non-symmorphic $\tilde{F}$ whose point group $\tilde{R}$ contains elements of order higher than 2.

B) $\tilde{F}$ whose point group $\tilde{R}$ has no subgroups $\tilde{R}^D$.

Case A1 (symmorphic $\tilde{F}$).

Here we have the following theorem:

(3.1.10) Those elements of $\tilde{D}_{\tilde{R}a}$ of a symmorphic $\tilde{F}$ for which $t_{\alpha}(R) = 0$ constitute a subgroup $\tilde{Q}$ of index 2 of $\tilde{D}_{\tilde{R}a}$, and, hence, $\tilde{Q}$ is a subgroup of index 4 of $\tilde{F}$.

To prove (3.1.10) we first observe that $\tilde{Q}$ is a group; in fact the product of two elements with $t_{\alpha}(R) = 0$ gives an element with $t_{\alpha}(R) = 0$ because (since $\tilde{D}_{\tilde{R}a}$ is a space group)
Rt\alpha = t_b. To show that \tilde{Q} is a subgroup of index 2 of \tilde{D}_{Ra} let us multiply any two elements of \tilde{D}_{R\alpha}, (R_1 | t_\alpha + t_a) and (R_2 | t_\alpha + t_b). The product is always of the form (R_1R_2 | t_c) because Rt_b = t_c and Rt_\alpha = t_\beta (the last equation follows from the fact that if Rt_\alpha = t_d one would have t_\alpha = R^{-1}t_d which would violate the condition that the lattice of \tilde{D}_{Ra} is invariant with respect to \tilde{R}), or in other words, the product belongs to \tilde{Q}.

Hence, according to theorem (2.2.7), the subgroup \tilde{Q} of \tilde{D}_{Ra} is of index 2.

From the above proof of (3.1.10) it also follows:

(3.1.11) The lattice of \tilde{Q} is identical with the lattice \tilde{T}D of \tilde{D}_{R\alpha} and the point group of \tilde{Q} is a subgroup \tilde{R}D of index 2 of \tilde{R}. In other words: the general element of \tilde{Q} is of the form (R_a | t_a) where R_a \in \tilde{R}D and t_a \in \tilde{T}D.

Theorems (3.1.10) and (3.1.11) imply that the elements of \tilde{F} can be arranged into left cosets relative to \tilde{Q} as follows:

\[
\begin{align*}
0^{th} \text{ coset} & \quad (E \mid 0)(R_a \mid t_a) \\
1^{st} \text{ coset} & \quad (E \mid t_\alpha)(R_a \mid t_a) \\
2^{nd} \text{ coset} & \quad (R_\alpha \mid 0)(R_a \mid t_a) \\
3^{rd} \text{ coset} & \quad (R_\alpha \mid t_\alpha)(R_a \mid t_a)
\end{align*}
\]

From (3.1.12) it is immediately apparent that

(3.1.13) the 0^{th} and the 3^{rd} coset constitute the group \tilde{D}_{R\alpha} from which we have started out;

(3.1.14) the 0^{th} and the 2^{nd} coset also constitute a
group, which is of the kind \tilde{D}_{Ro}.
(3.1.15) the 0th and the 1st coset also constitute a group, which is of the kind \( \tilde{D}_T \).

The following rule for constructing all the \( \tilde{D}_{F\alpha} \)'s of a given symmorphic \( \tilde{F} \) will then be valid.

(3.1.16) Take the set \( ^\wedge \) of all those elements \((R_a \mid t_a)\) of the symmorphic space group \( \tilde{F} \) for which \( R_a \) belongs to some specified \( \tilde{R}^D \) and \( t_a \) belongs to some specified \( \tilde{T}^D \) of \( \tilde{T} \) which has the same holohedry as \( \tilde{T} \). The set \( ^\wedge \) then will form a group which will be necessarily a subgroup of index 4 of \( \tilde{F} \), and every subgroup \( \tilde{Q} \) of any subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \) will be identical with one of the groups obtained in this way by taking all such pairs \( \tilde{R}^D \), \( \tilde{T}^D \). Also the set consisting of the elements of the 0th and 3rd cosets will necessarily form a group. This is either a subgroup \( \tilde{D}_{R\alpha} \) or \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \). The latter case occurs when all the \( t_\alpha \) can be transformed away, or, in other words, when the group, formed by the 0th and 3rd cosets of \( \tilde{F} \) relative to \( \tilde{Q} \) is not properly different (see Section 2.3) from the group formed by the 0th and 2nd cosets of \( \tilde{F} \) relative to \( \tilde{Q} \).

That \( ^\wedge \) forms a group follows immediately by considering the product of two arbitrary elements of \( ^\wedge \).

\[
(R_a \mid t_a)(R_b \mid t_b) = (R_a \mid t_a + R_at_b).
\]

In fact, \( R_at_b = t_c \) in view of (3.1.8).

That the set constituted by the 0th and 3rd cosets is a group follows similarly by considering the product of two arbitrary elements of the set. This product necessarily belongs to the set, again because of (3.1.8) which implies \( R_\alpha t_\alpha = t_\beta \).
$R_a t_\alpha = t_\gamma$ (a fact already used in the proof of (3.1.10)).

Digression.

Rule (3.1.16) can be slightly extended so as to become a rule for obtaining all the subgroups $\tilde{D}$ of index 2 of a given symmorphic space group $\tilde{F}$ if its point group $\tilde{R}$ has subgroups $\tilde{R}^D$. This possibility readily follows from (3.1.14) and (3.1.15), and the rules (3.1.4) and (3.1.9) specialized to the case of a symmorphic $\tilde{F}$.

The extended rule (3.1.16) is:

(3.1.17) Take the set $\Lambda$ of all those elements $(R_a|t_a)$ of the symmorphic space group $\tilde{F}$ for which $R_a$ belongs to some specified $\tilde{R}^D$ and $t_a$ belongs to some specified $\tilde{T}^D$ of $\tilde{F}$, which has the same holohedry as $\tilde{T}$. The set $\Lambda$ is a group, which will be necessarily a subgroup $\tilde{Q}$ of index 4 of $\tilde{F}$, and the elements of $\tilde{F}$ can be arranged into cosets as in the (3.1.12). The elements of the $0^{th}$ and $1^{st}$ coset will then necessarily form a subgroup $\tilde{D}_T$ of $\tilde{F}$. Similarly the elements of the $0^{th}$ and $2^{nd}$ coset will form a subgroup $\tilde{D}_{R0}$ and those of the $0^{th}$ and $3^{rd}$ coset will form a subgroup $\tilde{D}_{R\alpha}$. By taking all possible pairs $\tilde{R}^D, \tilde{T}^D$ of $\tilde{F}$, one will obtain in this way all possible subgroups $\tilde{D}_T, \tilde{D}_{R0}$ and $\tilde{D}_{R\alpha}$ of a symmorphic space group $\tilde{F}$ (if its point group $\tilde{R}$ has subgroups $\tilde{R}^D$).

Case A2 and A3 (non-symmorphic $\tilde{F}$).

The procedure for constructing the $\tilde{D}_{R\alpha}$'s in Case A1 is based on the validity of theorem (3.1.10). This theorem is not always valid in the case of non-symmorphic space groups.
Consequently, the procedure cannot be always used for non-symmorphic space groups without some modification.

If a non-symmorphic space group $\tilde{F}$ has a point group which does not contain elements of order higher than 2 theorem (3.1.10) is still valid although its proof is somewhat more complicated. For a non-symmorphic space group $\tilde{F}$ whose point group contains some elements of order higher than 2 theorem (3.1.10) may occasionally be valid but is not valid in general. That is why we distinguish between Case A2 and A3.

Before considering the two cases separately we will repeat some very well-known properties of the elements of a non-symmorphic space group.

Let $(r | r(R) + t)$ be an element of some $\tilde{F}$. If $R$ is a proper rotation or a reflection in a plane a non-primitive translation $\tau(R)$ along the rotation axis in the first case, and parallel to the plane of reflection in the second case, cannot be transformed away by shifting the origin of the coordinate system. In all other cases there is always a translation by means of which $\tau(R)$ can be transformed away. It will be convenient to say that $\tau(R)$ is a "true" non-primitive translation when it cannot be transformed away. Different elements of a space group may have different true $\tau(R)$. In such a case the non-primitive translation of an element $R$ will not in general consist of the true $\tau(R)$ but also of an additional non-primitive translation which could be transformed away from that particular element although not from all the other elements
of the group. We will call this additional non-primitive transla-
tion the "apparent" non-primitive translation of $R$.

Case A2 (non-symmorphic $\tilde{F}$ belonging to the monoclinic or
orthorhombic system).

The analogue of theorem (3.1.10) in this case is as
follows:

(3.1.18) Let $\tilde{F}$ be a non-symmorphic space group whose
point group has no elements of order higher than 2. Those
elements $(R | \tau(R)+t_\alpha(R)+t_b)$ of a subgroup $\tilde{D}_{R\alpha}$ of $\tilde{F}$ for which
$\tau(R) = 0$ form a subgroup of index 2 of $\tilde{D}_{R\alpha}$, and, hence a
subgroup $\tilde{Q}_{\tau\alpha}$ of index 4 of $\tilde{F}$.

The proof of (3.1.18) consists of two parts.

First we show that $\tau(R)$ cannot be equal to $t_\alpha/2$. In
fact, if $\tau(R)$ were a true non-primitive translation and were
equal to $t_\alpha/2$ then equations

$$Rt_a = t_b \quad \text{and} \quad Rt_\alpha = T_\beta$$

would imply

$$(R | \tau(R)+t_\alpha(R)+t_a)^2 = (E | t_\beta),$$

which would contradict the fact that the lattice of $\tilde{D}_{R\alpha}$ is $\tilde{T}_D$, and hence does not contain $t_\beta$. On the other hand, $\tau(R)$
cannot be an apparent non-primitive translation equal to $t_\alpha/2$ because if it did this would imply the presence in $\tilde{D}_{R\alpha}$ of some
other element with a true non-primitive translation equal to
$t_\alpha/2$. We conclude that $\tau(R)$ can only be zero or equal to a
half of a primitive translation of $T^D$.

The result implies next that the product of two elements of $\tilde{D}_{R\alpha}$ $(R_1 | \tau(R_1) + t_\alpha(R_1) + t_a)$ and $(R_2 | \tau(R_2) + t_\alpha(R_2) + t_b)$ is of the form $(R_1R_2 | \tau(R_1R_2) + t_c)$ if both $t_\alpha(R_1)$ and $t_\alpha(R_2)$ are zero or both different from zero. The first part of this statement shows that the elements with $t_\alpha(R) = 0$ form a group, the second part together with theorem (2.2.7) shows that the group is a subgroup of index 2 of $\tilde{D}_{R\alpha}$, and, hence, a subgroup $\tilde{Q}_{\tau_\circ}$ of index 4 of $\tilde{F}$.

Obviously,

(3.1.19) the lattice of $\tilde{Q}_{\tau_\circ}$ is identical with the lattice $\tilde{T}^D$ of $\tilde{D}_{R\alpha}$ and the point group of $\tilde{Q}_{\tau_\circ}$ is a subgroup $\tilde{N}^D$ of index 2 of $\tilde{N}$. In other words the general element of $\tilde{Q}_{\tau_\circ}$ is of the form $(R_a | \tau(R_a) + t_a)$ where $R_a \in \tilde{N}^D$, $t_a \in \tilde{T}^D$.

From (3.1.18) and (3.1.19) it follows that the elements of $\tilde{F}$ can be arranged into left cosets relative to $\tilde{Q}_{\tau_\circ}$ as follows:

- **0th coset** $(E | 0)(R_a | \tau(R_a) + t_a)$
- **1st coset** $(E | t_\alpha)(R_a | \tau(R_a) + t_a)$

(3.1.20)

- **2nd coset** $(R_\alpha | \tau(R_\alpha))(R_a | \tau(R_a) + t_a)$
- **3rd coset** $(R_\alpha | \tau(R_\alpha) + t_\alpha)(R_a | \tau(R_a) + t_a)$.

The 0th and the 3rd coset constitute the group $\tilde{D}_{R\alpha}$ from which we have started out; the 0th and the 2nd coset constitute a group of the kind $\tilde{D}_{R_0}$; the 0th and the 1st coset constitute a group of the kind $\tilde{N}_T$. 
Hence, just as in the case of a symmorphic space group \( \tilde{F} \), we have the following rule for constructing all the \( \tilde{D}_{R^\alpha} \)'s of a given non-symmorphic space group \( \tilde{F} \) whose point group does not contain elements of order higher than 2:

\[
(3.1.21) \text{Take the set } \Theta \text{ of all those elements of } \tilde{F} \text{ for which } R_a \text{ belongs to some fixed subgroup } R^D \text{ of } \tilde{R} \text{ and } t_a \text{ belongs to some subgroup } T^D \text{ of } \tilde{T} \text{ which has the same holohedry as } \tilde{T}. \text{ If } \Theta \text{ is a group, then it will be necessarily a subgroup of index 4 of } \tilde{F} \text{ and every subgroup } \tilde{Q}_{\tau_\alpha} \text{ of any subgroup } \tilde{D}_{R^\alpha} \text{ of } \tilde{F} \text{ will be identical with one of the groups obtained in that way by considering all such pairs } R^D \text{ and } T^D. \text{ Arrange the elements of } \tilde{F} \text{ into cosets relative to } \Theta = \tilde{Q}_{\tau_\alpha} \text{ as in (3.1.20). If the elements of the 0th and 2nd coset form a group this group is a subgroup } \tilde{D}_{R^0} \text{ of } \tilde{F}, \text{ if the elements of the 0th and 3rd coset form a group this group is a subgroup } \tilde{D}_{R^X} \text{ of } \tilde{F}.
\]

In the case of symmorphic space groups we could generalize the analogous rule (3.1.16) for constructing all the \( \tilde{D}_{R^\alpha} \)'s so as to obtain the extended rule (3.1.17) for constructing all the \( \tilde{D} \)'s of a given symmorphic \( \tilde{F} \).

In the present case such an extension is not possible. The reason for this difference is that while every symmorphic \( \tilde{D}_T \) can always be regarded as consisting of the 0th and 1st coset in (3.1.12), this is not always so in the case of a non-symmorphic \( \tilde{D}_T \). Hence, in the present case of a non-symmorphic \( \tilde{F} \), the analogue of the extended rule need not give all the
\(\tilde{D}_T\)'s for some \(\tilde{F}\)'s, and, in fact, it does not, as will be shown in Section 3.2. Of course, this does not invalidate the completeness of our general procedure, according to which all \(\tilde{D}_T\)'s of a given \(\tilde{F}\) can be obtained by using (3.1.4).

**Case A3** (non-symmorphic \(\tilde{F}\) belonging to the tetragonal, trigonal, hexagonal or cubic system).

We will consider in turn non-symmorphic space groups \(\tilde{F}\) belonging to the four systems just enumerated.

**Tetragonal system; \(\tilde{F}\) whose lattice is plain (P).**

Here we have to distinguish between two cases:

Either the lattice \(\tilde{T}^D\) of a \(\tilde{D}_{R\alpha}\) of \(\tilde{F}\) is such that the basic primitive translation \(t_{\alpha}\) belonging to \(\tilde{T} - \tilde{T}^D\) is perpendicular to the 4-fold axis, or the lattice \(\tilde{T}^D\) is such that \(t_{\alpha}\) is parallel to the 4-fold axis.

In the former case the procedure developed for Case A2 will obviously be valid without any change. In other words, a theorem analogous to (3.1.18) which ensures the existence of a subgroup \(\tilde{Q}_{\tau_0}\) will be valid, and all subgroups \(\tilde{D}_{R\alpha}\) of this kind will be obtained from the rule (3.1.21).

In the latter case, that is in the case of \(\tilde{D}_{R\alpha}\)'s in which \(t_{\alpha}\) is parallel to the 4-fold axis, the procedure must be modified. Let us call the subgroups \(\tilde{D}_{R\alpha}\) of this kind the "standard" subgroups of \(\tilde{F}\). A standard subgroup \(\tilde{D}_{R\alpha}\) has thus the property that the basic primitive translation of its lattice \(\tilde{T}^D\) along the direction of the 4-fold axis is twice as large as that of \(\tilde{T}\) along the same direction.
Let \((R \uparrow \tau(R) + t_\alpha \downarrow (R) + t_a)\) be an element of a standard subgroup \(\tilde{D}_{R\alpha}\) of \(\tilde{F}\). If \(R\) is of order 2 then a true non-primitive translation must be of the form \(t_b/2\) whereas an apparent non-primitive translation can be of the form \(t_\alpha/2\) provided that the element for which it is a true non-primitive translation is of order 4. If \(\tau(R_4)\) of an element \(R_4\) of order 4 has a component \(\xi(R_4)\) which is a true non-primitive translation of \(R_4\) then
\[
4 \xi(R_4) = m 2 t_\alpha
\]
or
\[
\xi(R_4) = \frac{m t_\alpha}{2}
\]
where \(m\) is either 0 or 1.

Hence:

(3.1.22) Only those tetragonal space groups \(\tilde{F}\) which contain the element 4 or the element 4\(_2\) can have standard subgroups \(\tilde{D}_{R\alpha}\).

(Here we have used, for convenience, the notation of the "International Tables", and we shall do that occasionally in the remainder of this section.)

It is easy to see that if \(\tilde{F}\) contains the element 4 a theorem analogous to (3.1.18) which ensures the existence of a subgroup \(\tilde{Q}_{t_0}\) again will be valid, and all subgroups \(\tilde{D}_{R\alpha}\) will be obtained from the rule (3.1.21).

If, on the other hand, \(\tilde{F}\) contains the element 4\(_2\) then this element must become either 4\(_1\) or 4\(_3\) in a standard subgroup
\[ \tilde{D}_\alpha \text{ of } \tilde{F}. \] It will be 41 or 43 depending on whether \( t_\alpha (R_4) = 0 \) or \( t_\alpha (R_4) = t_\alpha \). One has then the two following theorems:

(3.1.23) If \( \tilde{F} \) contains the element 42 then those elements of a standard subgroup \( \tilde{D}_\alpha \) of \( \tilde{F} \) for which \( t_\alpha (R) = 0 \) do not form a group; in other words, subgroups \( \tilde{Q}_\alpha \) do not exist in this case.

The validity of this theorem follows immediately from the fact that, since \( \tau (R_4) = t_\alpha /2 \),

\[ (R_4 |\tau (R_4)+t_a)^2 = (R_4^2 | t_\alpha+t_b), \]

which contradicts the requirement that the square of each element of \( \tilde{Q}_\alpha \) must belong to \( \tilde{Q}_\alpha \).

(3.1.24) If \( \tilde{F} \) contains the element 42 then each standard subgroup \( \tilde{D}_\alpha \) of \( \tilde{F} \) has subgroups \( \tilde{Q}_\alpha \) of index 2 with elements of the form \( (R_a|\tau (R_a)+t_\alpha (R_a)+t_a) \) where \( t_\alpha (R_a) = t_\alpha \) for some \( R_a \).

The validity of this theorem follows from the fact that the point group \( \tilde{\Gamma} \) of \( \tilde{F} \) has by assumption subgroups of index 2, and from the fact that the product of any two elements of the form \( (R_\alpha |\tau (R_\alpha)+t_\alpha (R_\alpha)+t_a) \) is necessarily of the form \( (R_a|\tau (R_a)+t_\alpha (R_a)+t_b) \).

From (3.1.24) follows:

(3.1.25) The lattice of a subgroup \( \tilde{Q}_\alpha \) of a group \( \tilde{D}_\alpha \) is identical with the lattice \( \tilde{D}^D \) of \( \tilde{D}_\alpha \) and the point group of \( \tilde{Q}_\alpha \) is a subgroup \( \tilde{R}^D \) of index 2 of \( \tilde{\Gamma} \).

Theorem (3.1.24) also implies that the elements of an \( \tilde{F} \) containing the element 42 can be arranged into left cosets.
relative to \( \tilde{Q}_\tau \alpha \) as follows:

\[
\begin{align*}
0\text{th coset} & \quad (E \circ (R_a | \tau(R_a) + t_\alpha(R_a) + t_a)) \\
1\text{st coset} & \quad (E \circ t_\alpha(R_a | \tau(R_a) + t_\alpha(R_a) + t_a)) \\
2\text{nd coset} & \quad (R_\alpha | \tau(R_\alpha) + t_\alpha(R_a) + t_a) \\
3\text{rd coset} & \quad (R_\alpha | \tau(R_\alpha) + t_\alpha(R_a) + t_\alpha(R_a) + t_a).
\end{align*}
\]

(3.1.26)

The 0\text{th} and the 3\text{rd} coset, and the 0\text{th} and the 2\text{nd} coset constitute groups \( \tilde{D}_{R\alpha} \); the 0\text{th} and the 1\text{st} coset constitute a group of the kind \( \tilde{D}_T \).

Hence, we have the following rule for constructing all the standard \( \tilde{D}_{R\alpha} \)'s of a given non-symmorphic \( \tilde{F} \) which contains 4\text{2}:

(3.1.27) Take the set \( \Sigma \) of elements

\( (R_a | \tau(R_a) + t_\alpha(R_a) + t_a) \) of \( \tilde{F} \) such that \( R_a \) belongs to some fixed subgroup \( \tilde{R}^D \) of \( \tilde{R} \), \( t_a \) belongs to some subgroup \( \tilde{T}^D \) of \( \tilde{T} \) which has the same holohedry as \( \tilde{T} \) and whose basic primitive translation along the 4-fold axis is twice the basic primitive translation of \( \tilde{T} \) along the same direction and \( t_\alpha(R_4^2) = t_\alpha \).

If \( \Sigma \) is a group, then it will be necessarily a subgroup of index 4 of \( \tilde{F} \), and every subgroup \( \tilde{Q}_\tau \alpha \) of any subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \) will be identical with one of the groups obtained in that way by considering all possible pairs of \( \tilde{R}^D \) and \( \tilde{T}^D \). Arrange the elements of \( \tilde{F} \) into cosets relative to \( \Sigma = \tilde{Q}_\tau \alpha \) as in (3.1.26). If the elements of the 0\text{th} and 2\text{nd} coset form a group this group is a subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \). Similarly if the elements of the 0\text{th} and 3\text{rd} coset form a group this group is
a subgroup \( \tilde{D}_R \alpha \) of \( \tilde{F} \).

**Tetragonal system: \( \tilde{F} \) whose lattice is body-centered (I).**

As is well known in these space groups besides the elements of the second order there can be only the elements 4 or 4\(_1\) and their powers.

Because of the condition (3.1.8) requiring \( \tilde{T} \) and \( \tilde{T}^D \) to have the same holohedry, only one kind of \( \tilde{T}^D \) has to be considered in this case (for the proof of this statement see Section 3.3), namely a plain lattice \( \tilde{T}^D \) whose elements are the translations

\[
(\varepsilon|2n_1a_1 + n_2(a_2 + a_3) + n_3(a_3 - a_2))
\]

here

\[
a_1 = \frac{a \cdot b \cdot c}{2}, \quad a_2 = \frac{a + b - c}{2}, \quad a_3 = \frac{a - b + c}{2},
\]

and

\[
t_\alpha = \frac{a + b + c}{2}.
\]

If \( \tilde{F} \) contains the element 4, the situation is the same as in the case of a tetragonal \( \tilde{F} \) with a plain lattice discussed before: a subgroup \( \tilde{Q}_{\tau_0} \) of \( \tilde{D}_R \alpha \) exists, and rule (3.1.21) can be used for constructing all \( \tilde{D}_R \alpha \)'s.

If \( \tilde{F} \) contains the element 4\(_1\) then this element must be either 4\(_1\) or 4\(_3\) in a subgroup \( \tilde{D}_R \alpha \) of \( \tilde{F} \). It will be 4\(_1\) or 4\(_3\) depending on whether \( t_\alpha (R_4) = 0 \) or \( t_\alpha (R_4) = t_\alpha \).
One then proves as in the case of a tetragonal $\widetilde{F}$ with a plain lattice the validity of two theorems which differ from (3.1.23) and (3.1.24) only by replacing "4₂" by "4₁" and omitting the word "standard", and hence shows that the elements of $\widetilde{F}$ can be arranged as in (3.1.26). We then obtain the following rule for finding all the $\widetilde{D}_{R\alpha}$'s of an $\widetilde{F}$ having a tetragonal body-centered lattice and containing the element 4₁:

(3.1.28) Take the set $\times$ of elements

$$(R_a | \tau(R_a) + t_\alpha(R_a) + t_a)$$

of $\widetilde{F}$ such that $R_a$ belongs to some fixed subgroup $\widetilde{R}D$ of $\widetilde{R}$, $t_a$ belongs to the subgroup $\widetilde{T}D$ of $\widetilde{T}$ which has the same holohedry as $\widetilde{T}$ and $t_\alpha (R_4 2) = t_\alpha$. If $\times$ is a group, then it will be necessarily a subgroup of index 4 of $\widetilde{F}$, and every subgroup $\widetilde{Q}_\tau \alpha$ of any subgroup $\widetilde{D}_{R\alpha}$ of $\widetilde{F}$ will be identical with one of the groups obtained in that way by considering all possible pairs of $\widetilde{R}D$ and $\widetilde{T}D$. Arrange the elements of $\widetilde{F}$ into cosets relative to $\times = \widetilde{Q}_\tau \alpha$ as in (3.1.26). If the elements of the 0th and 2nd coset form a group this group is a subgroup $\widetilde{D}_{R\alpha}$ of $\widetilde{F}$. Similarly, if the elements of the 0th and 3rd coset form a group this group is a subgroup $\widetilde{D}_{R\alpha}$ of $\widetilde{F}$.

**Trigonal system and hexagonal system.**

The procedure for finding all the $\widetilde{D}_{R\alpha}$'s of an $\widetilde{F}$ of either of these two systems is the same as in the case of the tetragonal system except for some obvious modifications.

**Trigonal system; $\widetilde{F}$ whose lattice is hexagonal.**

In this case because of the holohedry condition (3.1.8)
all subgroups $\hat{\tilde{D}}_R$ of $\tilde{F}$ have the same lattice which has along the 3-fold axis a basic primitive translation twice as large as that of $\tilde{T}$ along the same direction. (All $\hat{\tilde{D}}_R \alpha$'s are thus "standard subgroups" in the sense in which this term has been used in the tetragonal case.) Let us call $t_\alpha$ the basic primitive translation of $\tilde{T}$ along the trigonal axis, that of $\tilde{T}^D$ in the same direction will be $2t_\alpha$.

As is well known in a space group $\tilde{F}$ of the trigonal system the true non-primitive translation for a rotation $R_3$ of order 3 can only be 0, 1/3 or 2/3 of the basic primitive translation along the axis (the corresponding elements of $\tilde{F}$ are $3$, $3_1$ and $3_2$). Thus in a subgroup $\hat{\tilde{D}}_R \alpha$ of a space group $\tilde{F}$ the true non-primitive translation for the rotation of order 3 will be $0$, $\frac{1}{3}2t_\alpha$, $\frac{2}{3}2t_\alpha$ and $0$, $\frac{2}{3}2t_\alpha$, $\frac{1}{3}2t_\alpha = \frac{1}{3}2t_\alpha^{(\text{mod} \ 2t_\alpha)}$ for its square respectively. Hence:

(3.1.29) A space group of the trigonal system which contains the element 3 can only have subgroups $\hat{\tilde{D}}_R \alpha$ which contain that element. A space group which contains $3_2$ has only subgroups $\hat{\tilde{D}}_R \alpha$ which contain the element $3_1$. A space group which contains $3_1$ has only subgroups $\hat{\tilde{D}}_R \alpha$ which contain the element $3_2$.

From (3.1.29) it follows that, if $\tilde{F}$ contains the element 3, a theorem analogous to (3.1.18) ensuring the existence of a subgroup $\tilde{Q}_\alpha$ will be valid, and the rule (3.1.21) can be used for obtaining all $\hat{\tilde{D}}_R \alpha$'s in this case, just as in the analogous tetragonal case.
Again, because of (3.1.29), the two following theorems, analogous to (3.1.23) and (3.1.24) can be proved in the same way as in the tetragonal case:

(3.1.30) If $\tilde{F}$ contains $3_1$ or $3_2$, those elements of $\tilde{D}_R\alpha$ for which $t_\alpha(R) = 0$ do not form a group; in other words subgroups $\tilde{Q}_{\tau\alpha}$ do not exist in this case.

(3.1.31) If $\tilde{F}$ contains $3_1$ or $3_2$, then each subgroup $\tilde{D}_R\alpha$ has subgroups $\tilde{Q}_{\tau\alpha}$.

By the same argument as in the tetragonal case we have then the following rule for constructing all the $\tilde{D}_R\alpha$'s for the trigonal case:

(3.1.32) Take the set $\Psi$ of elements

$$(Ra | \tau (Ra) + t_\alpha (Ra) + t_\alpha)$$

of $\tilde{F}$ such that $Ra$ belongs to some fixed $\tilde{R}^D$ of $\tilde{R}$, $t_\alpha$ belongs to the subgroup $\tilde{T}^D$ of $\tilde{T}$ which has the same holohedry as $\tilde{T}$ and $t_\alpha(Ra) = t_\alpha$ for $R_3$ or for its inverse. If $\Psi$ is a group then it will be necessarily a subgroup of index 4 of $\tilde{F}$, and every subgroup $\tilde{Q}_{\tau\alpha}$ of any subgroup $\tilde{D}_R\alpha$ of $\tilde{F}$ will be identical with one of the groups obtained in that way by considering all possible pairs of $\tilde{R}^D$ and $\tilde{T}^D$. Arrange the elements of $\tilde{F}$ into cosets relative to $\Psi = \tilde{Q}_{\tau\alpha}$ as in (3.1.26). If the elements of the 0th and 2nd coset form a group, this group is a subgroup $\tilde{D}_R\alpha$ of $\tilde{F}$. Similarly, if the elements of the 0th and 3rd coset form a group this group is a subgroup $\tilde{D}_R\alpha$ of $\tilde{F}$.

**Trigonal system:** $\tilde{F}$ whose lattice is rhombohedral.

In this case it turns out (see Section 3.2) that the conditions for the existence of $\tilde{D}_R$'s of a non-symmorphic $\tilde{F}$
are never satisfied; in other words, a trigonal non-symmorphic \( \tilde{F} \) with a rhombohedral lattice does not have subgroup \( \tilde{D}_R \).

**Hexagonal system**

In this case, because of the holohedry condition (3.1.8), all subgroups \( \tilde{D}_R \) of an hexagonal space group \( \tilde{F} \) have the same lattice \( \tilde{T}^D \) which has the basic primitive translation along the 6-fold axis twice as large as that of \( \tilde{T} \) along the same direction.

A rotation \( R_6 \) of order 6 can have a non-primitive translation equal to 0, 1/6, 2/6, 3/6, 4/6, 5/6 of the basic primitive translation along the direction of its axis. The corresponding elements of \( \tilde{F} \) are: 6, 61, 62, 63, 64, 65.

If \( 2t_\alpha \) is the basic primitive translation along the 6-fold axis of a \( \tilde{D}_R \), the possible true non-primitive translations of \( R_6 \) in \( \tilde{D}_R \) are: \( 0, \frac{1}{6} 2t_\alpha, \frac{2}{6} 2t_\alpha, \frac{3}{6} 2t_\alpha, \frac{4}{6} 2t_\alpha, \frac{5}{6} 2t_\alpha \). Hence:

(3.1.33) If \( \tilde{F} \) contains the element \( (R_6 | 0) \) a subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \) can contain either the element \( (R_6 | 0) \) or the element \( (R_6 | t_\alpha) = (R_6 | \frac{3}{6} 2t_\alpha) \), that is, in the first case \( D_{R\alpha} \) contains the element 6, in the second case contains the element 63. If \( \tilde{F} \) contains \( (R_6 | \frac{1}{6} 2t_\alpha) \), a subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \) can contain either \( (R_6 | \frac{1}{6} 2t_\alpha) \) or \( (R_6 | \frac{2}{6} t_\alpha + t_\alpha) = (R_6 | \frac{4}{6} 2t_\alpha) \). In the first case \( \tilde{D}_{R\alpha} \) contains the element 61, in the second case contains the element 64. Finally if \( \tilde{F} \) contains \( (R_6 | \frac{4}{6} t_\alpha) \), a subgroup \( \tilde{D}_{R\alpha} \) of \( \tilde{F} \) may contain either \( (R_6 | \frac{2}{6} 2t_\alpha) \) or \( (R_6 | \frac{1}{6} t_\alpha + t_\alpha) = (R_6 | \frac{5}{6} 2t_\alpha) \). In the first case \( \tilde{D}_{R\alpha} \) contains
6_2, in the second case \( \tilde{D}_{R\alpha} \) contains 6_5.

From (3.1.33) it follows that if \( \tilde{F} \) contains the element 6 a \( \tilde{Q}_\tau \) will exist just as in the analogous case of tetragonal and trigonal system, and the rule (3.1.21) can be used for obtaining all the \( \tilde{D}_{R\alpha} \)'s of \( \tilde{F} \).

In all other cases two theorems analogous to (3.1.23), (3.1.24) and (3.1.30), (3.1.31) will be valid, and either a \( \tilde{Q}_\tau \) will exist or no \( \tilde{D}_R \) will exist at all. From the discussion given in the following section it follows that no \( \tilde{D}_R \) can exist if \( \tilde{F} \) contains elements 6_1, 6_3 or 6_5. If \( \tilde{F} \) contains 6_2 or 6_4 then a rule for constructing all \( \tilde{D}_{R\alpha} \)'s of \( \tilde{F} \) can be formulated. It will be analogous to (3.1.28).

**Cubic system.**

The problem of constructing all \( \tilde{D}_{R\alpha} \)'s of \( \tilde{F} \) in this case can be easily settled using the rules derived previously, and the discussion of this case can be very brief.

Point groups of the space groups of the cubic system always have elements of order 3 or of order 3 and 4 besides elements of order 2.

The rotations of order 3 never have true non-primitive translations. If the lattice of a space group is plain a rotation of order 4 may have a true non-primitive translation equal to 0, 1/4, 2/4 or 3/4 of the basic primitive translation along the 4-fold axis. The corresponding elements of \( \tilde{F} \) are 4, 4_1, 4_2, 4_3. If the lattice is body-centered a rotation of order 4 may appear in the space group
only as 4 or 4₁. Thus what has been said for space groups of the tetragonal system holds for space groups of the cubic system which contain 4, 4₁, 4₂ or 4₃.

For space groups of the cubic system which do not contain elements of order 4 the theory is essentially the same as for the case of non-symmorphic space groups with no elements of order higher than 2.

B) A whose point group ⤾ has no subgroups ⤾⁰

There are only two point groups which do not have subgroups ⤾⁰. They are: 3 and 23.

The symmorphic space groups with these point groups have only subgroups ⤾₀ which can be constructed by means of rule (3,1.9). The space group F23 does not have any subgroup of index 2 at all.

The non-symmorphic space groups are P3₁, P3₂, P2₁3, I2₁3. Of them P2₁3 does not have subgroups ⤾ᵣ because the conditions (see Section 3.2) under which the elements (R |τ(R)+tₐ) of P2₁3 would form a group are not satisfied. Of the others, P3₁ has a subgroup P3₂, and P3₂ has a subgroup P3₁. Both subgroups have a lattice which differs from that of the original space group because its basic primitive translation along the 3-fold axis is twice as large as that of the original lattice in that same direction. Both subgroups contain elements with tₐ(R) = tₐ. In fact, P3₁ contains the element (R₃ |τ(R₃)+t) with R₃ a rotation of order
3 and \( \tau(R_3) = \frac{1}{3} \alpha \) and its subgroup \( \tilde{D}_{R^A} \) contains
\( (R_3 | \tau(R_3) + t_\alpha + t_a) = (R_3 | \frac{1}{3} \alpha + t_a) \); \( P3_2 \) contains
\( (R_3 | \tau(R_3) + t) \) with \( \tau(R_3) = \frac{2}{3} \alpha \) and its subgroup \( \tilde{D}_{R^A} \) contains
\( (R_3 | \frac{1}{3} \alpha + t_a) \) and \( (R_3 | 2 \alpha + t_a) = (R_3^2 | 2 \alpha + t_a) \).
The group \( I213 \) has as a subgroup \( \tilde{D}_{RO} \) the space group \( P2_13 \).

**SECTION 3.2**

We have proved quite generally in Section 3.1 that all the subgroups \( \tilde{D}_T, \tilde{D}_{RO} \) and \( \tilde{D}_{R^A} \) of a symmorphic space group \( \tilde{F} \) can be obtained from the subgroups \( \tilde{Q} \) of \( \tilde{F} \) of the form
\( (R_a | t_{\alpha}) \) except in the case of an \( \tilde{F} \) whose point group does not have subgroups of index 2 and that all the \( \tilde{Q} \)'s can be constructed by means of the rule (3.1.16). In the exceptional cases just mentioned the subgroups of index 2 of \( \tilde{F} \) are necessarily of the kind \( \tilde{D}_{RO} \) or \( \tilde{D}_{R^A} \) and can be all obtained using rule (3.1.9) in the symmorphic case, and have been all enumerated in the non-symmorphic case.

We have also proved that all the subgroups \( \tilde{D}_{RO} \) and \( \tilde{D}_{R^A} \) of a non-symmorphic space group \( \tilde{F} \) whose point group does not contain elements of order higher than 2 can be obtained from the subgroups \( \tilde{Q}_{\tau_0} \) of \( \tilde{F} \) of the form \( (R_a | \tau(R_a) + t_a) \) and that all the subgroups \( \tilde{D}_{RO} \) and \( \tilde{D}_{R^A} \) of a non-symmorphic space group \( \tilde{F} \) whose point group contains elements of order higher than 2 as well as elements of order 2 can be obtained from the subgroups \( \tilde{Q}_{\tau_0} \) and \( \tilde{Q}_{\tau^A} \) of \( \tilde{F} \). However, in the case of non-symmorphic space groups \( \tilde{F} \) we have only given necessary
conditions for the sets $\Lambda$, $\Theta$, $\Sigma$, $\times$, $\Psi$ of elements of various $\tilde{F}$ to form subgroups $\tilde{Q}_{\tau_0}$ or $\tilde{Q}_{\tau_\alpha}$. In this section we show what the necessary and sufficient conditions are for these sets to form groups $\tilde{Q}_{\tau_0}$ or $\tilde{Q}_{\tau_\alpha}$, and also what the necessary and sufficient conditions are for the pairs of cosets relative to $\tilde{Q}_{\tau_0}$ or $\tilde{Q}_{\tau_\alpha}$ to form groups $\tilde{D}_{R_0}$ or $\tilde{D}_{R_\alpha}$.

We will deal first (Case A2) with non-symmorphic space groups whose point groups do not contain elements of order higher than 2. We will deal (Case A3) with the non-symmorphic space groups whose point groups contain elements of order higher than 2 later on.

**Case A2**

Here we have the following theorem:

(3.2.1) The set $\Theta$ (defined in (3.1.21)) of elements $(R_a | \tau(R_a) + t_a)$ of a given space group $\tilde{F}$ is a group if and only if

(3.2.2) $R_a t_a \in \tilde{T}^D$,

(3.2.3) $\tau(R_a R_b) = \tau(R_a) + R_a \tau(R_b) + t_c$,

for any choice of $R_a$, $R_b$ and $t_a$.

These conditions simply follow from the fact that $\Theta$ is necessarily a group if the product of any two elements of $\Theta$, $(R_a | \tau(R_a) + t_a)$ and $(R_b | \tau(R_b) + t_b)$, belongs to $\Theta$.

It should be noticed that the product just mentioned would also be an element of $\Theta$ if the following conditions
were satisfied:

\[ R_a t_b \in \tilde{T} - \tilde{T}^b, \]

\[ \tau(R_a R_b) = \tau(R_a) + R_a \tau(R_b) + t_\alpha, \]

for any choice of \( R_a, R_b \) and \( t_b \). However, these conditions cannot be satisfied for an arbitrary choice of \( R_a, R_b \) and \( t_b \).

(Take, for example, \( t_b = 0 \).)

From conditions (3.2.2) and (3.2.3) one obtains:

(3.2.4) If \( \Theta \) is a group then it is a space group whose point group is a \( \tilde{D} \) and whose lattice is a \( \tilde{T}^D \), and, as a subgroup of \( \tilde{F} \), it is a subgroup \( \tilde{Q}_{\tau_0} \) of index 4.

Before we state the conditions under which the 0th and 2nd coset of (3.1.21) form a group, we shall first have to see of which form the elements of the 2nd coset are in the case of a non-symmorphic space group whose point group has no elements of order higher than 2.

(3.2.5) Since the 2nd coset can be written as \( (R_\alpha | \tau(R_\alpha)) (R_a | \tau(R_a) + t_a) \), its general element can be either \( (R_\beta | \tau(R_\beta) + t_b) \) or \( (R_\beta | \tau(R_\beta) + t_\beta) \) depending on whether the conditions

(3.2.6)

\[ R_\alpha t_\alpha \in \tilde{T}^b, \]

(3.2.7)

\[ \tau(R_\alpha R_\alpha) = \tau(R_\alpha) + R_\alpha \tau(R_\alpha) + t_c, \]
or the conditions

\begin{align}
(3.2.8) \quad R_\alpha t_\alpha & \in \mathcal{T} - \mathcal{T}^b, \\
(3.2.9) \quad \tau(R_\alpha R_\alpha) & = \tau(R_\alpha) + R_\alpha \tau(R_\alpha) + t_\gamma,
\end{align}

are satisfied for any choice of $R_\alpha$, $R_\alpha$ and $t_\alpha$. However, it is obvious that condition (3.2.8) is not satisfied for any $t_\alpha$. (Take, for example, $t_\alpha = 0$.) It follows that the elements of the 2nd coset can only be of the form

\[ (R_\rho | \tau(R_\rho) + t_\beta). \]

Requiring that the product of any two elements of the set consisting of the 0th and 2nd coset is again an element of the set one obtains:

\begin{align}
(3.2.10) \quad \text{The 0th coset } (R_\alpha | \tau(R_\alpha) + t_\alpha) \text{ and the 2nd coset } (R_\rho | \tau(R_\rho) + t_\beta) \text{ form a group if and only if} \\
(3.2.11) \quad \tau(R_\alpha R_\rho) & = \tau(R_\alpha) + R_\alpha \tau(R_\rho) + t_\delta, \\
(3.2.12) \quad \tau(R_\gamma R_\rho) & = \tau(R_\gamma) + R_\gamma \tau(R_\rho) + t_\delta,
\end{align}

for an arbitrary choice of $R_\alpha$, $R_\rho$ and $R_\gamma$.

Combining (3.2.6), (3.2.7), (3.2.11) and (3.2.12) one obtains:

\begin{align}
(3.2.13) \quad \text{The 0th and 2nd coset form a group if and only if}
\end{align}
(3.2.14) \[ R \, t_{\alpha} \in \tilde{T}^D \]

(3.2.15) \[ \tau(R, R) = \tau(R) + R \tau(R) + t_b \]

for any \( R, R_1 \) and \( R_2 \) belonging to \( \tilde{R} \) and any \( t_a \) belonging to \( \tilde{T}^D \).

Condition (3.2.14) is nothing else but the condition (3.1.8) which states that \( \tilde{T}^D \) must have the same holohedry as \( \tilde{T} \). Hence (3.2.13) can be reformulated as follows:

(3.2.16) The 0th and 2nd coset form a group if and only if \( \tilde{T} \) and \( \tilde{T}^D \) have the same holohedry, and

(3.2.17) \[ \tau(R, R) = \tau(R) + R \tau(R) + t_b \]

for any \( R_1 \) and \( R_2 \) belonging to \( \tilde{R} \).

Consider now the 0th and 3rd coset.

(3.2.18) The elements of the 3rd coset \( (R_\alpha | \tau(R_\alpha) + t_\alpha)(R_\alpha | \tau(R_\alpha) + t_\alpha) \) can be either of the form \( (R_B | \tau(R_B) + t_B) \) or \( (R_B | \tau(R_B) + t_B) \) depending on whether the conditions

(3.2.19) \[ R_\alpha t_\alpha \in \tilde{T}^D \]

(3.2.20) \[ \tau(R_\alpha R_\alpha) = \tau(R_\alpha) + R_\alpha \tau(R_\alpha) + t_c \]

or the conditions

(3.2.21) \[ R_\alpha t_\alpha \in \tilde{T} \cdot \tilde{T}^B \]

(3.2.22) \[ \tau(R_\alpha R_\alpha) = \tau(R_\alpha) + R_\alpha \tau(R_\alpha) + t_c \]
are satisfied for an arbitrary choice of $R_\alpha$, $R_\delta$ and $t_\alpha$.

However it is obvious that condition (3.2.21) is not always satisfied. (Take for example, $t_\alpha = 0$.). It follows that the elements of the 3rd coset can only be of the form $(R_B | \tau(R_B) + t_B)$.

Using the same arguments as in the previous case one obtains:

(3.2.23) The 0th coset $(R_a | \tau(R_a) + t_a)$ and the 3rd coset $(R_B | \tau(R_B) + t_B)$ form a group if and only if

\begin{align*}
(3.2.24) \quad \tau(R_\alpha R_\beta) &= \tau(R_\alpha) + R_\alpha \tau(R_\beta) + t_\delta, \\
(3.2.25) \quad \tau(R_\gamma R_\delta) &= \tau(R_\delta) + R_\gamma \tau(R_\delta) + t_\epsilon,
\end{align*}

for an arbitrary choice of $R_\alpha$, $R_\beta$ and $R_\gamma$.

Combining (3.2.19), (3.2.20), (3.2.24) and (3.2.25) one obtains:

(3.2.26) The 0th and 3rd coset form a group if and only if

\begin{align*}
(3.2.27) \quad &R \in \widetilde{T}^D, \\
(3.2.28) \quad &\tau(R, R_1) = \tau(R_1) + R_1 \tau(R_1) + t_b,
\end{align*}

for an arbitrary choice of $R$, $R_1$ and $R_2$ belonging to $\tilde{R}$ and $t_a$ belonging to $\tilde{T}^D$. 
Using again the concept of holohedry, (3.2.26) can be reformulated as follows:

\[ (3.2.29) \] The 0\textsuperscript{th} and 3\textsuperscript{rd} coset form a group if and only if \( \tilde{T} \) and \( \tilde{T}^D \) have the same holohedry, and

\[ (3.2.30) \quad \tau(R, R_\xi) = \tau(R_\xi) \tau(R, \tau(R_\xi) \cdot t_b), \]

for any \( R_1 \) and \( R_2 \) belonging to \( \tilde{R} \).

As one can see from (3.2.13) and (3.2.26) the conditions under which the 0\textsuperscript{th} and 2\textsuperscript{nd} coset, and the 0\textsuperscript{th} and 3\textsuperscript{rd} coset form groups are identical.

Hence:

\[ (3.2.31) \text{ If for a given } \tilde{Q}_{\nu_0} \text{ of a space group } \tilde{F} \text{ whose point group does not have elements of order higher than } 2 \text{ a subgroup } \tilde{D}_{\nu_0} \text{ of } \tilde{F} \text{ exists, then there exists also a subgroup } \tilde{D}_{\nu_0} \text{ of } \tilde{F} \text{ with the same lattice } \tilde{T}^D \text{ as } \tilde{D}_{\nu_0}. \]

Conversely:

\[ (3.2.32) \text{ If a } \tilde{D}_{\nu_0} \text{ with a given } \tilde{T}^D \text{ does not exist, then the } \tilde{D}_{\nu_0} \text{ with the same lattice does not exist either.} \]

Case A3

We now consider those non-symmorphic space groups \( \tilde{F} \) whose point groups contain elements of order higher than 2 as well as elements of order 2.

If the subgroup \( \tilde{T}^D \) of \( \tilde{T} \) is such that the basic primitive translation \( t_{\alpha} \) belonging to \( \tilde{T} \) but not to \( \tilde{T}^D \) is perpendicular to the axis of higher order then in order to
construct the $\tilde{D}$'s of an $\tilde{F}$ one has to consider the set $\Theta$ of (3.2.1), and the theory of Case A2 applies without any change. However if the translation $t_\alpha$ defined above is parallel to the axis of higher order one has to consider the set $\Phi$ of elements $(R_a | \tau(R_a)+t_\alpha(R_a)+t_a)$ of $\tilde{F}$ which will be the set $\Xi$ of (3.1.27) if $\tilde{F}$ has the plain lattice and contains the element 42, the set $\chi$ of (3.1.28) if $\tilde{F}$ has the body-centered lattice and contains the element 41, etc.

(3.2.33) A set $\Phi$ of elements $(R_a | \tau(R_a)+t_\alpha(R_a)+t_a)$ of $\tilde{F}$ is a group if and only if

$$R_\alpha t_\alpha \in \tilde{T}^P,$$  

(3.2.34) and

$$\tau (R_a R_b)+t_\alpha (R_a R_b)=\tau (R_\alpha)+t_\alpha (R_\alpha)+R_\alpha [\tau (R_b)+t_\beta (R_b)+t_\gamma],$$  

(3.2.35)

for an arbitrary choice of $R_a, R_b$ and $t_a$.

These conditions follow from the fact that $\Phi$ is necessarily a group if the product of any two elements of $\Phi$, $(R_a | \tau(R_a)+t_\alpha(R_a)+t_a)$ and $(R_b | \tau(R_b)+t_\alpha(R_b)+t_b)$, belongs to $\Phi$. Also they are the only conditions under which $\Phi$ is a group. In fact, the conditions

$$R_\alpha t_\alpha \in \tilde{T}^{-P},$$  

(3.2.35)

$$\tau (R_a R_b)+t_\alpha (R_a R_b)=\tau (R_\alpha)+t_\alpha (R_\alpha)+R_\alpha [\tau (R_b)+t_\beta (R_b)+t_\gamma],$$  

(3.2.36)
under which $\phi$ would be a group too, are not satisfied for an arbitrary choice of $R_a$, $R_b$ and $t_a$.

(3.2.37) If $\phi$ is a group it is a space group whose point group is a $\tilde{R}^D$ and whose lattice is a $\tilde{T}^D$, and as a subgroup $\tilde{\mathcal{F}}$ of $\tilde{F}$, is of index 4.

We now consider the pairs of 0th and 2nd coset, and of 0th and 3rd coset. However, before doing that we will have to see of which form the elements of the 2nd and of the 3rd coset are.

We know that the 2nd coset consists of the elements $(R_\alpha|\tau(R_\alpha))(R_a|\tau(R_a)+t_\alpha(R_a)+t_a)$. Its general element can be either $(R_B|\tau(R_B)+t_\alpha(R_B)+t_b)$ or $(R_B|\tau(R_B)+t_\alpha(R_B)+t_B)$ depending on whether the conditions

\begin{align}
(3.2.38) & \quad R_\alpha t_\alpha \in \tilde{T}^D, \\
(3.2.39) & \quad \tau(R_\alpha R_a)+t_\alpha(R_\alpha R_a)=\tau(R_\alpha)+R_\alpha[R_\alpha(R_a)+t_\alpha(R_a)]+t_c,
\end{align}

or the conditions

\begin{align}
(3.2.40) & \quad R_\alpha t_\alpha \in \tilde{T}-\tilde{T}^D, \\
(3.2.41) & \quad \tau(R_\alpha R_a)+t_\alpha(R_\alpha R_a)=\tau(R_\alpha)+R_\alpha[R_\alpha(R_a)+t_\alpha(R_a)]+t_c,
\end{align}

are satisfied for an arbitrary choice of $R_a$, $R_\alpha$, and $t_a$. However, it is obvious that (3.2.40) is not always satisfied. (Take, for example, $t_a = 0$).
(3.2.42) The 0\textsuperscript{th} coset \((R_a|\tau(R_a)+t_{\alpha}(R_a))\) and the 2\textsuperscript{nd} coset \((R_B|\tau(R_B)+t_{\alpha}(R_B)+t_B)\) form a group if and only if

\[
(3.2.43) \quad \tau(R_aR_B) + t_{\alpha}(R_aR_B) = \tau(R_a) + t_{\alpha}(R_a) + R_{\alpha}[\tau(R_B)+t_{\alpha}(R_B)] + t_{\alpha}
\]

\[
(3.2.44) \quad \tau(R_lR_p) + t_{\alpha}(R_lR_p) = \tau(R_l) + t_{\alpha}(R_l) + R_{\alpha}[\tau(R_p)+t_{\alpha}(R_p)] + t_{\alpha}
\]

for an arbitrary choice of \(R_a\), \(R_B\) and \(R\).

Combining (3.2.38), (3.2.39), (3.2.43) and (3.2.44) one obtains:

(3.2.45) The 0\textsuperscript{th} and 2\textsuperscript{nd} coset form a group if and only if

\[
(3.2.46) \quad R_{t_{\alpha}} \in \tilde{T}^D
\]

\[
(3.2.47) \quad \tau(R_1R_2) + t_{\alpha}(R_1R_2) = \tau(R_1) + t_{\alpha}(R_1) + R_{\alpha}[\tau(R_2)+t_{\alpha}(R_2)] + t_{\alpha}
\]

for any \(R\), \(R_1\) and \(R_2\) belonging to \(\tilde{T}\) and any \(t_{\alpha}\) belonging to \(\tilde{T}^D\).

Again one can reformulate (3.2.45), (3.2.46) and (3.2.47) as follows:
(3.2.48) The 0th and 2nd coset form a group if and only if \( \bar{T} \) and \( \bar{T}^D \) have the same holohedry and if (3.2.47) holds for an arbitrary choice of \( R_1 \) and \( R_2 \) of \( \bar{R} \).

Consider now the 0th and 3rd coset. Using the same arguments as in the previous case one can easily show that the general element of the 3rd coset is of the form
\[
(R_B | \tau(R_B) + t_\alpha(R_B) + t_\beta) \quad \text{and that the 0th and 3rd coset form a group if and only if}
\]
(3.2.49) \( R \cdot \bar{t}_\omega \in \bar{T}^D \)

(3.2.50) \( \tau(R_1, R_2) + \bar{t}_\alpha(R_1, R_2) = \tau(R_1) + \bar{t}_\alpha(R_2) \)
\[
+ R_1 [ \tau(R_2) + \bar{t}_\alpha(R_2) ] + \bar{t}_b
\]
for an arbitrary choice of \( R, R_1 \) and \( R_2 \) belonging to \( \bar{T} \) and \( \bar{T}^D \) or, in other words:

(3.2.51) The 0th and 3rd coset form a group if and only if \( \bar{T} \) and \( \bar{T}^D \) have the same holohedry and if (3.2.50) holds.

(3.2.52) If the 0th and 2nd coset and the 0th and 3rd coset form groups, these are space groups and as subgroups of \( \bar{F} \) they are both \( \bar{D}_{R, \alpha} \).

Since the 0th and 2nd coset, and the 0th and 3rd coset form groups under the same conditions, if the first pair of cosets constitutes a group the second one does too.
Conversely, if the first pair of cosets is not a group, the second pair is not a group either.

Condition (3.2.50) is never satisfied for non-symmorphic space groups which have the plain lattice and the elements $4_1, 4_3, 6_1, 6_3, 6_5$, that is why in Section 3.1 we said that these space groups do not have standard $\tilde{D}_{R\alpha}$.

Similarly, condition (3.2.30) is never satisfied for non-symmorphic trigonal space groups with a rhombohedral lattice; that is why we have not discussed this case in Section 3.1.

This completes the discussion of the problem of formulating and proving the rules for constructing all subgroups of index 2 of all space groups.

Digression

Our method of constructing the subgroups $\tilde{D}$ of $\tilde{F}$ is based on the observation that, apart from exceptional cases, these subgroups have in turn subgroups of index 2 which are subgroups of index 4 ($\tilde{Q}, \tilde{Q}_{T\alpha}$ or $\tilde{Q}_{T\gamma\alpha}$) of $\tilde{F}$, and that these subgroups of index 4 of $\tilde{F}$ can be very easily found (roughly speaking, by taking a "half" of the point group $\tilde{R}$ of $\tilde{F}$ and a "half" of the lattice $\tilde{T}$ of $\tilde{F}$).

The exceptional cases are, as we have seen, of two kinds. The point group $\tilde{R}$ may not have subgroups $\tilde{R}^D$ of index 2; this situation has been dealt with by means of rule (3.1.9), and by considering the four exceptional non-symmorphic $\tilde{F}$'s separately (end of Section 3.1): in both
cases no reference is made to the subgroups of index 4 of $\tilde{F}$. The other kind of exceptional situation arises for some non-symmorphic $\tilde{F}$'s; here some $\tilde{D}_T$, which can always be obtained from rule (3.1.4), cannot be obtained from any $\tilde{Q}_\tilde{\gamma}$ or $\tilde{Q}_{\tilde{\gamma} \tilde{\alpha}}$ as pointed out explicitly in Section 3.1 in connection with the case of the non-symmorphic $\tilde{F}$'s of the monoclinic and orthorhombic systems. We shall examine here somewhat closer the reasons for this being so.

Consider first the case of the monoclinic and orthorhombic systems ($\tilde{F}$ whose point group does not have elements of order higher than 2).

If $\tilde{F}$ is symmorphic, no difficulty arises:

(3.2.53) All subgroups $\tilde{D}_T$ of a symmorphic $\tilde{F}$ can be obtained from some $\tilde{Q}$ of $\tilde{F}$.

The validity of this theorem is an immediate consequence of the following theorem which is a result of the survey of lattices in Section 3.3:

(3.2.54) With the exception of the face-centered cubic lattice every lattice $\tilde{T}$ has at least one subgroup $\tilde{T}^D$ of index 2 with the same holohedry as $\tilde{T}$. In fact, from (3.2.54), it immediately follows:

(3.2.55) With the exception of the face-centered cubic lattice every lattice $\tilde{T}$ has at least one subgroup of index 2 which is invariant under all the subgroups of index 2 of the holohedry of $\tilde{T}$ and its subgroups.

Hence:

(3.2.56) Each symmorphic $\tilde{F}$ of the monoclinic and
orthorhombic system has at least as many subgroups $\tilde{Q}$ of index 4 as there are subgroups $\tilde{R}^D$ of the point group $\tilde{R}$. In other words for every $\tilde{R}^D$ there is at least one subgroup $\tilde{Q}$ of $\tilde{F}$.

If $\tilde{F}$ is non-symmetric (for any system, not only monoclinic or orthorhombic) we have to take into account an additional circumstance:

(3.2.57) A necessary condition for a set $\Lambda$ of elements $(R_a, \tau(R_a) + t_a)$ of a non-symmetric space group $\tilde{F}$ to be a group is

$$R_{a}^{-1} \tau(R_{a}) + R_{a}^{-2} \tau(R_{a}) + \cdots + R_{a} \tau(R_{a}) + \tau(R_{a}) \in \tilde{T}^b$$

for all the elements of the set. Here $R_a$ is a proper or improper rotation of order $n$, and $R_a^k$ stands for the $k^{th}$ power of the rotation $R_a$.

There are only a few cases when for a given $\tilde{R}^D$ there are no subgroups $\tilde{T}^D$ such that (3.2.57) is not satisfied. Obviously this happens when the elements of $\Lambda$ have true non-primitive translations in all three directions of the edges of the non-primitive unit cell of $\tilde{T}$. More precisely:

(3.2.58) If in a non-symmetric space group $\tilde{F}$ with no elements of order higher than 2 there are two perpendicular diagonal glide plane reflections (e.g. Pnnm), or two perpendicular diamond glide plane reflections (e.g. Fddd), or three screw rotations of order 2 about perpendicular axes (e.g. Pnma) or a screw rotation of order 2 and a diagonal glide plane reflection perpendicular to it, then (3.2.3) is not satisfied.
for a $\Theta$ containing such pairs of operations whatever $\tilde{T}^D$ may be.

Hence we conclude:

(3.2.59) Not all the subgroups $\tilde{D}_T$ of every non-symmorphic group $\tilde{F}$ belonging to the monoclinic or orthorhombic system can be obtained from some $\tilde{Q}_{\tau'}$.

However, we repeat, this is not a difficulty since all the subgroups $\tilde{D}^T$ of any $\tilde{F}$ can be obtained by means of the rule (3.1.4).

In the case of the trigonal, hexagonal and cubic systems the situation is quite similar.

If $\tilde{F}$ is symmorphic, no difficulty arises, and (3.2.53) remains true.

In the case of non-symmorphic $\tilde{F}$ a difficulty arises because condition (3.2.57) when applied to subgroups $\tilde{Q}_{\tau\alpha}$ becomes

(3.2.60) $R_{\alpha}^{-1}[\tau(R_{\alpha})+t_{\alpha}(R_{\alpha})]+R_{\alpha}^{-1}[\tau(R_{\alpha})+t_{\alpha}(R_{\alpha})]+\cdots+[\tau(R_{\alpha})+t_{\alpha}(R_{\alpha})] \in \tilde{T}^p$

and this condition is not satisfied by all those elements of order 2 whose true non-primitive translation has a component along the axis of higher order. (This occurs, e.g. in the groups $P4_2cm$, $P3c1$).

Hence:

(3.2.61) For a non-symmorphic space group whose point group contains elements of order higher than 2 there is not
necessarily a $Q_{\tau^\alpha}$ for every $R^D$ of $\tilde{R}$.

Hence:

(3.2.62) Not all the subgroups $\tilde{D}_T$ of a non-symmorphic space group $\tilde{F}$ whose point group contains elements of order higher than 2 can be obtained from some $Q_{\tau^\alpha}$ and therefore they have to be obtained by means of (3.1.4).

SECTION 3.3

From the previous section it is clear that in order to construct the subgroups $\tilde{D}$ of a given space group $\tilde{F}$ one has to find all the different subgroup $T^D$ of the lattice $\tilde{T}$ of $\tilde{F}$ and the subgroups $R^D$ of its point group $\tilde{R}$.

A complete list of subgroups $R^D$ of each of the 32 point groups is given in "The International Tables for X-Ray Crystallography" (1952).

We now turn to the problem of finding all the different subgroups $T^D$ of a given lattice $\tilde{T}$.

Two lattices are called "different" if they do not consist of the same set of points which are the end-points of primitive translation vectors. As is well known, two sets of three basic primitive translations generate the same lattice if and only if there exists an integral unimodular square matrix which transforms one set into the other. Hence, if such a matrix does not exist the two sets of basic primitive translations generate different lattices. Using this criterion it is easy to enumerate all the different subgroups
\( \tilde{T}^D \) of a given \( \tilde{T}^D \); there are at most seven of them.

Let \( a_1, a_2 \) and \( a_3 \) be the basic primitive translations of the lattice \( \tilde{T}^D \). Obviously the group \( \tilde{T}_{D_1}^D \) consisting of the primitive translations \( t_a = 2n_1a_1+n_2a_2+n_3a_3 \) with \( n_1, n_2 \) and \( n_3 \) integers constitutes a subgroup of index 2 of \( \tilde{T}^D \). Five other subgroups \( \tilde{T}^D \) can be obtained from it by permutation of \( a_1, a_2 \) and \( a_3 \) but only two of them are different among themselves and different from \( \tilde{T}_{D_1}^D \). They are the group \( \tilde{T}_{D_2}^D \) consisting of the primitive translations \( t_a = n_1a_1+2n_2a_2+n_3a_3 \) and the group \( \tilde{T}_{D_3}^D \) consisting of the primitive translations \( t_a = n_1a_1+n_2a_2+2n_3a_3 \). The group \( \tilde{T}_{D_4}^D \) consisting of the primitive translations \( t_a = 2n_1a_1+n_2(a_1+a_2)+n_3a_3 \) is also a subgroup of index 2 of \( \tilde{T}^D \) and again five other subgroups \( \tilde{T}^D \) can be obtained from it by all possible permutations of \( a_1, a_2 \) and \( a_3 \). Of them only two are different among themselves and different from \( \tilde{T}_{D_4}^D \). They can be chosen as the group \( \tilde{T}_{D_5}^D \) consisting of the primitive translations 
\[
t_a = 2n_1a_1+n_2a_2+n_3(a_1+a_3) 
\]
and the group \( \tilde{T}_{D_6}^D \) consisting of the primitive translations 
\[
t_a = n_1a_1+2n_2a_2+n_3(a_2+a_3). 
\]
Finally the group \( \tilde{T}_{D_7}^D \) consisting of the primitive translations \( t_a = 2n_1a_1+n_2(a_1+a_2)+n_3(a_1+a_3) \) is a subgroup of index 2 of \( \tilde{T}^D \) different from the six already defined.

There are no other subgroups of index 2 of \( \tilde{T}^D \). In fact any other set of primitive translations of \( \tilde{T}^D \) forming a group is a subgroup of \( \tilde{T}^D \) of index higher than 2.
We list here the seven subgroups of index 2 of a lattice $\tilde{T}$ whose basic primitive translations are $a_1, a_2$ and $a_3$:

\[
\tilde{T}_1 = (2a_1, a_2, a_3),
\]

\[
\tilde{T}_2 = (a_1, 2a_2, a_3),
\]

\[
\tilde{T}_3 = (a_1, a_2, 2a_3),
\]

\[
\tilde{T}_4 = (2a_1, a_1+a_2, a_3),
\]

\[
\tilde{T}_5 = (2a_1, a_2, a_1+a_3),
\]

\[
\tilde{T}_6 = (a_1, 2a_2, a_2+a_3),
\]

\[
\tilde{T}_7 = (2a_1, a_1+a_2, a_1+a_3).
\]

If there are relations between the vectors $a_1, a_2, a_3$ (which is always the case for systems different from the triclinic system), the number of different subgroups $\tilde{T}_D$ of a given $\tilde{T}$ will be less than seven. This point is discussed further in Chapter 4.

Of course, not every subgroup $\tilde{T}_D$ ($i = 1, 2...7$) of the lattice $\tilde{T}$ of a given space group $\tilde{F}$ satisfies condition (3.1.8) which require $\tilde{T}_D$ to have the same holohedry as $\tilde{T}$.

SECTION 3.4

In this section we shall give examples of the theory explained in the present chapter. We shall construct all the
subgroups $\mathbf{D}$ of the space groups $\text{P}4$, $\text{P}4_1$, $\text{P}4_2$ and $\text{P}4_3$ of the tetragonal system.

All these space groups have a plain lattice $\mathbf{P}$ with the basic primitive translations $a_1$, $a_2$ and $a_3$ which in this case are also the edges of the parallelopiped unit cell of $\mathbf{P}$, that is, $a_1 = a$, $a_2 = b$, $a_3 = c$. Also $a = b$ and $a = b = \gamma = 90^\circ$. From these relations it follows that the only subgroups of index 2 of the plain tetragonal lattice which have the same holohedry as the original lattice are of the type $\mathbf{D}_3^T$, $\mathbf{D}_4^T$ and $\mathbf{D}_7^T$.

All four space groups considered above have the point group $4$. This group consists of the elements

- $E$ - identity
- $C_{4z}^1$ - rotation about $z$-axis by $90^\circ$,
- $C_{4z}^2$ - rotation about $z$-axis by $180^\circ$,
- $C_{4z}^3$ - rotation about $z$-axis by $270^\circ$.

The elements $E$ and $C_{4z}^2$ constitute the only subgroup of index 2 of the point group 4.

We now consider each space group separately.

The space group $\text{P}4$ is symmorphic and consists of the following elements (we shall repeatedly use this phrase instead of a more correct phrase "has the following"
generating elements"):

\[(E | n_1 a + n_2 b + n_3 c), (C_{4z} | 0), (C_{4^2} | 0), (C_{4^3} | 0)\].

Let us consider the sets of elements

\[(E | n_1 a + n_2 b + 2n_3 c), (C_{4^2} | 0)\],

\[(E | 2n_1 a + n_2(a+b) + n_3 c), (C_{4^2} | 0)\],

\[(E | 2n_1 a + n_2(a+b) + n_3(a+c)), (C_{4^2} | 0)\].

Each of these sets is a group and a subgroup \(\tilde{Q}\) of \(P_4\). Call them \(\tilde{Q}_1\), \(\tilde{Q}_2\) and \(\tilde{Q}_3\) respectively. We then consider the 1st, 2nd and 3rd coset of \(P_4\) relative to each \(\tilde{Q}\), and see which of them form a group with \(\tilde{Q}\). Consider \(\tilde{Q}_1\) first. The cosets relative to \(\tilde{Q}_1\) are

0th coset \([(E | 0) | (E | n_1 a + n_2 b + 2n_3 c), (E | 0)(C_{4^2} | 0)\],

1st coset \([(E | c) | (E | n_1 a + n_2 b + 2n_3 c), (E | c)(C_{4^2} | 0)\],

2nd coset \([(C_{4^2} | 0) | (E | n_1 a + n_2 b + 2n_3 c), (C_{4^2} | 0)(C_{4^2} | 0)\],

3rd coset \([(C_{4^2} | c) | (E | n_1 a + n_2 b + 2n_3 c), (C_{4^2} | c)(C_{4^2} | 0)\].
The subgroup $\tilde{Q}_1$, which is the $0^{th}$ coset, together with the $1^{st}$ coset, constitutes a group which is the space group $P2$. This is a subgroup $\tilde{D}_T$ of $P4$ because it has the same lattice as $P4$ and because its point group is a $\tilde{R}^D$ of 4.

The subgroup $\tilde{Q}_1$, together with the $2^{nd}$ coset, constitutes a group which is the space group $P4$. This is a subgroup $\tilde{D}_R\alpha$ of $P4$ because it has the same point group as $P4$, a lattice which is a $\tilde{T}^D$ of the lattice $P$ of $P4$ and contains no elements with $t^\alpha$ which in this case is $c$.

Finally $\tilde{Q}_1$, together with the $3^{rd}$ coset, forms a group which is the space group $P4_2$. This is a subgroup $\tilde{D}_R\alpha$ of $P4$ because it has the same point group as $P4$, a lattice which is a $\tilde{T}^D$ of $P$ and elements with $t^\alpha = c$.

Clearly in this case the space groups $\tilde{D}_R\alpha$ and $\tilde{D}_R\alpha$ are properly different (in the sense defined in Section 2.3), or as we shall often say following the more customary terminology, "inequivalent".

Similarly the cosets of $P4$ relative to $\tilde{Q}_2$ are

\begin{align*}
0^{th} \text{ coset} & \quad (E | o)(E | 2n_1 a + n_2 (a+b) + n_3 c), (E | o)(C_{4z} | o) \\
1^{st} \text{ coset} & \quad (E | c)(E | 2n_1 a + n_2 (a+b) - n_3 c), (E | c)(C_{4z} | o) \\
2^{nd} \text{ coset} & \quad (C_{4z} | o)(E | 2n_1 a + n_2 (a+b) + n_3 c), (C_{4z} | o)(C_{4z} | o) \\
3^{rd} \text{ coset} & \quad (C_{4z} | c)(E | 2n_1 a + n_2 (a+b) - n_3 c), (C_{4z} | c)(C_{4z} | o).
\end{align*}
The 0th coset, which is $\tilde{Q}_2$, together with the 1st coset gives the space group P2, together with the 2nd, or the 3rd coset gives the space group P4. In this case $\tilde{R}_{Ro}$ and $\tilde{R}_{Rr}$ are equivalent (that is, not properly different).

Finally the cosets of P4 relative to $\tilde{Q}_3$ are

- 0th coset
  \[ (E|0)(E|2n,a+n_1(a+b)+n_2(a+c)), (E|0)(C_{4\hat{2}}|0) \]

- 1st coset
  \[ (E|c)(E|2n,a+n_1(a+b)+n_2(a+c)), (E|c)(C_{4\hat{2}}|0) \]

- 2nd coset
  \[ (C_{4\hat{2}}|0)(E|2n,a+n_1(a+b)+n_2(a+c)), (C_{4\hat{2}}|0)(C_{4\hat{2}}|0) \]

- 3rd coset
  \[ (C_{4\hat{2}}|c)(E|2n,a+n_1(a+b)+n_2(a+c)), (C_{4\hat{2}}|c)(C_{4\hat{2}}|0) \]

The 0th and 1st coset give the space group P2, the 0th and 2nd and the 0th and 3rd give the space group I4.

We now consider the space group P4$_1$. It consists of the elements

\[ (E|n_1a+n_2b+n_3c), (C_{4\hat{2}}|\frac{a}{2}), (C_{4\hat{2}}|\frac{c}{2}), (C_{4\hat{2}}|\frac{3c}{2}) \]
Let us consider the sets of elements

\[(E \mid 2n, a + n_x b + 2n_3 c), (C_{4z} \mid \frac{1}{2})\]

\[(E \mid 2n, a + n_x (a+b) + n_3 c), (C_{4z} \mid \frac{1}{2})\]

\[(E \mid 2n, a + n_x (a+b) + n_3 (a+c)), (C_{4z} \mid \frac{1}{2})\]

Only the second set is a group, a subgroup \(Q_{20}\) of \(P_4\). The cosets of \(P_4\) relative to this subgroup \(Q_{20}\) are

0th coset \((E \mid 0, 0, 0, 0) (E \mid 2n, a + n_x (a+b) + n_3 c), (E \mid 0, 0, 0, 0) (C_{4z} \mid \frac{1}{2})\)

1st coset \((E \mid a, 0, 0, 0) (E \mid 2n, a + n_x (a+b) + n_3 c), (E \mid a, 0, 0, 0) (C_{4z} \mid \frac{1}{2})\)

2nd coset \((C_{4z} \mid \frac{1}{2}) (E \mid 2n, a + n_x (a+b) + n_3 c), (C_{4z} \mid \frac{1}{2}) (C_{4z} \mid \frac{1}{2})\)

3rd coset \((C_{4z} \mid \frac{1}{2} + a) (E \mid 2n, a + n_x (a+b) + n_3 c), (C_{4z} \mid \frac{1}{2} + a) (C_{4z} \mid \frac{1}{2})\).

The 0th and 1st coset give the space group \(P_{21}\), the 0th and 2nd and the 0th and 3rd give the space group \(P_4\). There are no other subgroups \(D\) of \(P_{41}\).
The space group $P4_2$ consists of the elements

$$(E | n, a + n_2 b + n_3 c), (Cu_2 | \xi), (Cu_2^2 | 0), (Cu_2^3 | \xi)$$

Consider the sets of elements

$$(E | n, a + n_2 b + n_3 c), (Cu_2^2 | c)$$

$$(E | 2n, a + n_2(a+b) - n_3 c), (Cu_2^2 | 0)$$

$$(E | 2n, a + n_2(a+b) - n_3(a+c)), (Cu_2^2 | c)$$

They are all groups. The first and the third are subgroups $\tilde{Q}_{\tau \alpha}$ of $P4_2$, the second is a subgroup $\tilde{Q}_{\tau \alpha}$ of $P4_2$.

The cosets of $P4_2$ relative to the first subgroup $\tilde{Q}_{\tau \alpha}$ are

0th coset

$$\emptyset$$

1st coset

$$(E | c)(E | n, a + n_2 b + 2n_3 c), (E | c)(Cu_2^2 | c)$$

2nd coset

$$(Cu_2^2 | \xi)(E | n_2 a + n_2 b + 2n_3 c), (Cu_2^2 | \xi)(Cu_2^2 | c)$$

3rd coset

$$(Cu_2^2 | \xi + c)(E | n, a + n_2 b + 2n_3 c), (Cu_2^2 | \xi + c)(Cu_2^2 | c)$$
The 0th and 1st coset give the space group P2; the 0th and 2nd coset give the space group P41; the 0th and 3rd coset give the space group P43.

The cosets relative to the second subgroup \( \tilde{Q} \subset \) are

0th coset \((E | 0)(E | 2m, a + n, (a + b) - n_3 c), (E | 0)(C_{4z} \cdot z | 0)\)

1st coset \((E | a)(E | 2m, a + n, (a + b) + n_3 c), (E | a)(C_{4z} \cdot z | 0)\)

2nd coset \((C_{4z} | \frac{\pi}{2})(E | 2m, a + n, (a + b) + n_3 c), (C_{4z} | \frac{\pi}{2})(C_{4z} \cdot z | 0)\)

3rd coset \((C_{4z} | \frac{\pi}{2} + a)(E | 2m, a + n, (a + b) + n_3 c), (C_{4z} | \frac{\pi}{2} + a)(C_{4z} \cdot z | 0)\)

The 0th and 1st coset give the space group P2; the 0th and 2nd coset give the space group P42; the 0th and 3rd coset give the space group P42 again.

The cosets of P42 relative to the third subgroup of index 4 of P42 are

0th coset \((E | 0)(E | 2m, a + n, (a + b) + n_3 (a + c)), (E | 0)(C_{4z} \cdot z | c)\)

1st coset \((E | a)(E | 2m, a + n, (a + b) + n_3 (a + c)), (E | a)(C_{4z} \cdot z | c)\)

2nd coset \((C_{4z} | \frac{\pi}{2})(E | 2m, a + n, (a + b) + n_3 (a + c)), (C_{4z} | \frac{\pi}{2})(C_{4z} \cdot z | c)\)
3rd coset \( \left( C_{4z} | \frac{a}{2} + \alpha \right) (E | 2n, a + n_{z}(a + b) + n_{3}(a + c)), \left( C_{4z} | \frac{a}{2} \right) \left( C_{4z} | c \right) \).

The 0th and 1st coset give the space group \( P2 \); the 0th and the 2nd and the 0th and 3rd coset give both the space group \( I4_{1} \). There are no other subgroups \( \tilde{D} \) of \( P4_{2} \).

Finally we have to consider the non-symmorphic space group \( P4_{3} \). This consists of the elements

\([E | m, a + n_{v} b + n_{3} c], (C_{4z} | \frac{a}{2}), (C_{4z} | \frac{a}{2}), (C_{4z} | \frac{a}{2}) \).

Consider the following sets of elements:

\([E | m, a + n_{v} b + 2n_{3} c], (C_{4z} | \frac{a}{2}) \)

\([E | 2m, a + n_{v}(a + b) + n_{3} c], (C_{4z} | \frac{a}{2}) \)

\([E | 2m, a + n_{v}(a + b) + n_{3}(a + c)], (C_{4z} | \frac{a}{2}) \).

Of them only the second set is a group, a subgroup \( \tilde{Q}_{P} \) of \( P4_{3} \). The cosets of \( P4_{3} \) relative to this \( \tilde{Q}_{P} \) are

0th coset \( (E | 0)(E | 2m, a + n_{v}(a + b) + 4n_{3} c), (E | 0)(C_{4z} | \frac{a}{2}) \)

1st coset \( (E | a)(E | 2m, a + n_{v}(a + b) + n_{3} c), (E | a)(C_{4z} | \frac{a}{2}) \).
2nd coset \((C_{4z} | \frac{3\pi}{4}) (\bar{E} | 2n_1 a + n_2 (a + b) - n_3 c), (C_{4z} | \frac{3\pi}{4}) (\bar{C}_{4z} | \frac{\pi}{2})\)

3rd coset \((C_{4z} | \frac{3\pi}{4} + a) (\bar{E} | 2n_1 a + n_2 (a + b) - n_3 c), (C_{4z} | \frac{3\pi}{4} + a) (\bar{C}_{4z} | \frac{\pi}{2})\)

The 0th and 1st coset give the space group \(P2_1\); the 0th and 2nd and the 0th and 3rd coset give the space group \(P4_3\). The space group \(P4_3\) has no other subgroups \(\tilde{D}\).

NOTES TO CHAPTER 3

A systematic discussion of the problem of finding and classifying the subgroups (not necessarily of index 2) of a given space group was given many years ago by Hermann (1929). In particular, he has introduced the division of all subgroups of a given space group into two classes: "Klassengleiche Untergruppen" (which, in the case of the subgroups of index 2, correspond to our \(\tilde{D}_\text{R}'\)'s) and "Zellengleiche Untergruppen" (which correspond to our \(\tilde{D}_\text{T}'\)'s). However, Hermann was not specifically interested in the subgroups of index 2, and he has not considered the distinction between \(\tilde{D}_\text{Ro}'\)'s and \(\tilde{D}_\text{R}^\alpha\)'s which we have introduced in Section 3.1, nor has he noticed the important role played by subgroups of index 4 (our \(Q\), \(Q_{\sim 0}\) and \(Q_{\sim \alpha}\)).

The idea of combining a "half" of the elements of the point group of a space group with a "half" of the elements of its lattice for the case of symmorphic space groups (i.e. constructing our subgroup \(\tilde{Q}\)) is implicit in Zamorzaev (1957), who apparently has used the idea to obtain the magnetic space
groups for the case of symmorphic space groups. As no rules for constructing the $\tilde{D}$'s are formulated in his paper, and no proofs are given, it is difficult to say to what extent our method differs from his. The important case of non-symmorphic space groups is discussed by Zamorzaev in a few sentences.

The seven subgroups of index 2 of a lattice are listed in Zamorzaev's paper.

It is easy to see that the problem of finding all the subgroups $\tilde{D}H$ of an arbitrary group $\tilde{H}$ is equivalent to the problem of finding all alternating representations of $\tilde{H}$. In fact, the factor group $\tilde{H}/\tilde{D}H$ has only two representations: the identical representation, and the alternating representation. Hence, each subgroup $\tilde{D}H$ of $\tilde{H}$ will "engender" (the meaning of this term is explained in Lomont (1959), page 234) one alternating representation of $\tilde{H}$. Conversely, knowing all alternating representations of $\tilde{H}$, one can find all $\tilde{D}H$'s: for each alternating representation one finds the group $\tilde{D}H$ which engenders it by simply picking out from $\tilde{H}$ all those elements to which +1 corresponds in the alternating representation in question.

The equivalence of the two problems has been noticed for the case in which $\tilde{H}$ is a point group or a space group by Indenbom (1959) and Niggli (1959).
CHAPTER 4

MAGNETIC SPACE GROUPS AND THEIR PROPERTIES

SECTION 4.1

In this chapter we shall be dealing only with non-trivial MSGs.

For convenience we shall repeat here rule (2.2.8) specialized to the case of MSGs.

(4.1.1) In order to obtain all the non-trivial MSGs one has to consider all the space groups \( \tilde{F} \) which have subgroups \( \tilde{D} \) of index 2. Then for each \( \tilde{D} \) of each \( \tilde{F} \) one has to combine the elements of \( \tilde{D} \) with the identity \( E \) of \( \tilde{A} \) and the elements of the coset \( \tilde{F} - \tilde{D} \) with the element \( E' \) of \( \tilde{A} \). The set of all elements of \( \tilde{D}E \) and \( (\tilde{F} - \tilde{D})E' \) will then necessarily constitute a non-trivial MSG.

An MSG obtained in this way from a given \( \tilde{F} \) and \( \tilde{D} \) will be denoted by \( \tilde{M}(\tilde{D}) \).

As we have said in Section 3.1 in general a space group \( \tilde{F} \) has subgroups of index 2 of three kinds: \( \tilde{D}_T \), \( \tilde{D}_{Ro} \) and \( \tilde{D}_{R\alpha} \). From this and from (4.1.1) we conclude:

(4.1.2) The MSGs obtained from a given \( \tilde{F} \) are in general of three kinds: \( \tilde{M}_T \equiv \tilde{M}(\tilde{D}_T) \), \( \tilde{M}_{Ro} \equiv \tilde{M}(\tilde{D}_{Ro}) \) and \( \tilde{M}_{R\alpha} \equiv \tilde{M}(\tilde{D}_{R\alpha}) \). Since a subgroup \( \tilde{D}_T \) of \( \tilde{F} \) consists of the elements \( (R_a \tau (R_a) + t) \), where \( R_a \) belongs to some \( \tilde{R}^D \) of \( \tilde{R} \) and \( t \) belongs to \( \tilde{T} \), the corresponding MSG \( \tilde{M}_T \) consists of the unprimed elements \( (R_a \tau (R_a) + t) \) and of the primed elements \( (R_{\alpha} \tau (R_{\alpha}) + t)' \).
Similarly, since a subgroup \( \tilde{D}_{R_{O}} \) of \( \tilde{F} \) consists of the elements \((R|\tau(R)+t_{a})\) where \( R \) belongs to \( \tilde{R} \) and \( t_{a} \) belongs to a subgroup \( \tilde{T}^{D} \) of \( \tilde{T} \) with the same holohedry as \( \tilde{T} \), the corresponding MSG \( \tilde{M}_{R_{O}} \) consists of the unprimed elements \((R|\tau(R)+t_{a})\) and of the primed elements \((R|\tau(R)+t_{B})'\). Finally, since a subgroup \( \tilde{D}_{R_{\alpha}} \) of \( \tilde{F} \) consists of the elements \((R_{a}|\tau(R_{a})+t_{a})\) and \((R_{\alpha}|\tau(R_{\alpha})+t_{\alpha}+t_{a})\) where \( R_{a} \) belongs to some \( \tilde{R}^{D} \) of \( \tilde{R} \), \( R_{\alpha} \) belongs to \( \tilde{R} - \tilde{R}^{D} \), \( t_{a} \) belongs to some \( \tilde{T}^{D} \) which has the same holohedry as \( \tilde{T} \) and \( t_{\alpha} \) belongs to \( \tilde{T} - \tilde{T}^{D} \), the corresponding MSG \( \tilde{M}_{R_{\alpha}} \) consists of the unprimed elements \((R_{a}|\tau(R_{a})+t_{a})\) and \((R_{\alpha}|\tau(R_{\alpha})+t_{\alpha}+t_{a})\) and of the primed elements \((R_{a}|\tau(R_{a})+t_{B})'\) and \((R_{\alpha}|\tau(R_{\alpha})+t_{\alpha}+t_{B})'\).

In Section 2.1 we have defined magnetic lattices and magnetic point groups independently of MSGs. We will now define the magnetic lattice and the magnetic point group "belonging to" a given MSG and we will also briefly discuss their properties.

(4.1.3) We call the set of all primitive translations of an MSG \( \tilde{M} \) the magnetic lattice "belonging to" \( \tilde{M} \) (or the magnetic lattice "of" \( \tilde{M} \)). Obviously this set is a group and hence a subgroup of \( \tilde{M} \).

Let us introduce a useful convention: call "primed" those rotations or translations which appear only in primed elements of an MSG, and call "unprimed" those rotations or those translations which appear both in primed and unprimed elements of an MSG. Then we can say, according to (4.1.2):

(4.1.4) The magnetic lattice of an \( \tilde{M}_{T} \) consists of the unprimed translations \((E|t)\); the magnetic lattice of an \( \tilde{M}_{R_{O}} \) or an \( \tilde{M}_{R_{\alpha}} \) consists of the unprimed translations \((E|t_{a})\) and...
of the primed translations \((E | t_b)'\).

(4.1.5) The magnetic lattice of an MSG \(\tilde{M}\) is an invariant subgroup of \(\tilde{M}\).

This follows from (2.2.1), (2.2.2), (2.2.3) and from the fact that \(Rt_a\) belongs to \(T^D\) and \(Rt_\alpha\) belongs to \(T - T^D\) for any choice of \(R, t_a\) and \(t_\alpha\).

(4.1.6) We call the largest magnetic point group which leaves a magnetic lattice \(\tilde{T}_M\) invariant holohedry of \(\tilde{T}_M\).

We now come to the definition of magnetic point group "belonging to" a given MSG \(\tilde{M}\).

(4.1.7) The magnetic point group "belonging to" an MSG \(\tilde{M}\) is the set of either unprimed, or unprimed and primed rotations, which are the rotatory part of the elements of \(\tilde{M}\).

From (4.1.2), it follows:

(4.1.8) The magnetic point group belonging to an MSG \(\tilde{M}_T\) consists of a subgroup of index 2 of unprimed elements and a coset of primed elements. The magnetic point group belonging to an MSG \(\tilde{M}_{Ro}\) or \(\tilde{M}_R\) consists of unprimed elements only.

A complete list of all properly different MSGs with the exception of those belonging to the orthorhombic system is given at the end of this thesis (the list for the orthorhombic system is in preparation). The MSGs are arranged into families. In this respect our list differs from that given by Belov, Neronova, Smirnova (1957). The classification
of MSGs into families seems to be more useful from the physical point of view. The symbols used to denote the various properly different MSGs are those of Belov, Neronova, Smirnova. Each symbol consists of two parts (as in the case of the international symbols for ordinary space groups): the first part indicates the magnetic lattice of the MSG in question, the second part its magnetic point group and the non-primitive translations. The symbols for magnetic lattices and magnetic point groups are explained in Sections 4.2 and 4.3.

It should be mentioned that two families of MSGs consist of trivial magnetic space groups only: the family of F23, and the family of P2₁3. These are the only two space groups which do not have subgroups of index 2 at all. Each of the remaining 228 families consists of at least two members, but in general, of more than two. There are altogether 1491 properly different magnetic space groups.

**SECTION 4.2**

As we have said in Section 2.1, the ordinary or Bravais lattices are a special case of the magnetic lattices.

We define a class of magnetic lattices in analogy to the usual definition of a class of Bravais lattices (see, for example, Lomont (1959), page 198):

\[(4.2.1)\] Two magnetic lattices (with a lattice point at the origin) belong to the same class if one can be transformed into the other by means of a homogeneous linear transformation.
transformation which also transforms the holohedry of the one into the holohedry of the other, the term holohedry being used in the sense of (4.1.6).

There are 22 classes of non-trivial magnetic lattices (that is, magnetic lattices which are not ordinary lattices), so that altogether there are 36 classes of magnetic lattices. The reason for the existence of only 22 new magnetic lattices is that although, as we have said, an ordinary lattice \( T \) has in general seven different subgroups \( \tilde{T}^D \) of index 2, relations among the three basic primitive translations of \( \tilde{T} \) and the condition for every \( \tilde{T}^D \) to have the same holohedry as \( \tilde{T} \) reduce the number of \( \tilde{T}^D \)'s of a given \( \tilde{T} \) from which magnetic lattices are derived.

In the case of an ordinary lattice a primitive unit cell is defined as a parallelepiped with edges given by three basic primitive translations \( a_1, a_2, a_3 \).

The same definition holds for a non-trivial magnetic lattice, except that some, or all, basic primitive translations become primed.

In both cases (ordinary lattice and non-trivial magnetic lattice) the whole lattice can be reproduced by translation of the primitive unit cell through primitive translations. However, in the case of a non-trivial magnetic lattice the primitive translations will be either unprimed (for an MSG \( \tilde{M}_T \)) or unprimed and primed (for an MSG \( \tilde{M}_R \)).

This definition of the primitive unit cell is different in the case of MSGs \( \tilde{M}_R \) from the one often used in physical
applications. The usual definition is chosen such that the whole lattice can be obtained by translation of the primitive unit cell through unprimed primitive translations. Hence the volume of the primitive unit cell defined in this way may be a multiple of the primitive unit cell according to our definition.

As in the case of ordinary lattices it is possible to define a symmetric unit cell, but we shall not need this definition here.

To describe the various classes of magnetic lattices we shall use non-primitive unit cell whose edges $a$, $b$, $c$ will be taken along the conventional coordinate axes of each of the seven crystallographic systems; $a$, $b$, $c$ are primed or unprimed primitive translations.

At the end of this section we give a list of the 36 classes of magnetic lattices arranged into "families"; a "family" of magnetic lattices $\tilde{T}_M$ consists of an ordinary lattice $\tilde{T}$ and of all the magnetic lattices obtained from $\tilde{T}$ by means of rule (2.2.8) ($\tilde{H}$ in the rule is $\tilde{T}$ in the present case), and having the same holohedry as $\tilde{T}$.

Each family is arranged in this way: first the ordinary lattice, then the magnetic lattices (in general, one from each class) derived from it listed in the same order in which the seven subgroups $\tilde{T}_D^i$ of a lattice $\tilde{T}$ are arranged in Section 3.3.

An ordinary lattice is represented by means of its basic primitive translations expressed in terms of $a$, $b$ and $c$; a magnetic lattice is represented by means of three independent
primitive translations of its subgroup of unprimed elements (see list of subgroups $\mathbb{T}_i^{D_1}$ of a lattice $\mathbb{T}$ in Section 3.3).

The symbols introduced by Belov, Neronova and Smirnova (1955) are also given. These symbols are really not very suitable if the principle of a classification into families is adopted. Moreover two different symbols sometimes denote the same class of magnetic lattices (e.g. Class 12 and Class 19).

**List of classes of magnetic lattices**

**Triclinic system:** $a \neq b \neq c$, $a \neq b \neq \gamma \neq 90^\circ$.

1. $(a,b,c)$

2. $(a,b,2c)$

Obviously all the non-trivial magnetic lattices that one can derive from the lattices of the class P belong to the class $P_s$.

**Monoclinic system:** $a \neq b \neq c$, $\alpha = \gamma = 90^\circ \neq \beta$.

3. $(a,b,c)$

4. $(2a,b,c)$

5. $(a,2b,c)$

6. $(2a,a+b,c)$

$C_a$
Since we have taken the y-axis to be the unique axis, the magnetic lattices \((a, b, 2c)\) belong to the class \(P_a\), and the magnetic lattices \((a, 2b, b+c)\) belong to the class \(C_a\). The remaining different magnetic lattices derived from a lattice \(P\) or \(C\) belong to the class \(P_s\) of the triclinic system.

**Orthorhombic system:** \(a \neq b \neq c, \ \alpha = \beta = \gamma = 90^\circ\).

10. \((a, b, c)\)  
11. \((2a, b, c)\)  
12. \((2a, a+b, c)\)  
13. \((2a, a+b, a+c)\)  
14. \((a+b, b, c)\)  
15. \((2a+b, b, c)\)  
16. \((a+b, b, 2c)\)  
17. \((2a+b, b, a+b+c)\)
18. \( \left( \frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2} \right) \)  
19. \( \left( \frac{a+b}{2}, \frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2} \right) \)
\( \left( \frac{a+b}{2}, \frac{a+c}{2}, \frac{a+c}{2} + \frac{b+c}{2} \right) \)  
\( \left( \frac{a+b}{2}, \frac{a+c}{2}, \frac{a+c}{2} + \frac{b+c}{2} \right) \)

20. \( \left( \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a-b-c}{2} \right) \)  
21. \( \left( \frac{a+b+c}{2}, \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a+b+c}{2}, \frac{a-b-c}{2} \right) \)  
\( \left( \frac{a+b+c}{2}, \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a+b+c}{2}, \frac{a-b-c}{2} \right) \)  
\( \left( \frac{a+b+c}{2}, \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a+b+c}{2}, \frac{a-b-c}{2} \right) \)

The magnetic lattices \( \mathcal{C}_A \) belong to the class \( \mathcal{A}_c \).

The magnetic lattices derived from an orthorhombic lattice which do not belong to any of the classes listed above, belong to the class \( \mathcal{P}_s \) of the triclinic system.

**Tetragonal system:** \( a = b \neq c, \ \alpha = \beta = \gamma = 90^\circ \).

22. \( (a, b, c) \)  
23. \( (a, b, 2c) \)  
24. \( (2a, a+b, c) \)  
25. \( (2a, a+b, a+c) \)  
26. \( \left( \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a-b-c}{2} \right) \)  
27. \( \left( \frac{a+b+c}{2}, \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a+b+c}{2}, \frac{a-b-c}{2} \right) \)  
\( \left( \frac{a+b+c}{2}, \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a+b+c}{2}, \frac{a-b-c}{2} \right) \)
The magnetic lattices \((2a, b, c), (a, 2b, c)\) belong to the class \(P_s\) of the orthorhombic system.

The magnetic lattices \((2a, b, a+c), (a, 2b, b+c)\) belong to the class \(C_a\) of the orthorhombic system.

All the magnetic lattices derived from \(I\) with the exception of \(P_I\) belong to the class \(P_s\) of the triclinic system.

**Trigonal system:** \(a = b = c, \quad \alpha = \beta = \gamma = 120^\circ\).

28. \((a, b, c)\) \(R\)

29. \((2a, a+b, a+c)\) \(R_I\)

All the other magnetic lattices derived from a lattice \(R\) belong to the class \(P_s\) of the triclinic system.

**Hexagonal system:** \(a = b \neq c, \quad \alpha = \beta = 90^\circ, \quad \gamma = 120^\circ\).

30. \((a, b, c)\) \(P\)

31. \((a, b, 2c)\) \(P_c\)

All the other magnetic lattices derived from a lattice \(P\) belong to the class \(P_s\) of the triclinic system.

**Cubic system:** \(a = b = c, \quad \alpha = \beta = \gamma = 90^\circ\).

32. \((a, b, c)\) \(P\)

33. \((2a, a+b, a+c)\) \(P_s\)
34. \( \left( \frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2} \right) \)

35. \( \left( \frac{a+b+c}{2}, \frac{a+b-c}{2}, \frac{a-b-c}{2} \right) \)

36. \( \left( \frac{2a+b+c}{2}, \frac{a+b+c}{2} + \frac{a+b-c}{2}, \frac{a+b+c}{2} + \frac{a-b-c}{2} \right) \)

The magnetic lattices \((2a,b,c), (a,2b,c), (a,b,2c)\) belong to the class \(P_C\) of the tetragonal system; the magnetic lattices \((2a,a+b,c), (2a,b,a+c), (a,2b,b+c)\) belong to the class \(P_C\) of the tetragonal system.

The magnetic lattices \(\left( \frac{a+b}{2}, \frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2} \right), \left( \frac{a+b}{2}, \frac{a+c}{2}, \frac{a+b}{2}, \frac{b+c}{2} \right)\) and \(\left( \frac{a+b}{2}, \frac{a+b}{2}, \frac{a+c}{2}, \frac{b+c}{2} \right)\), belong to the class \(A_C\) of the orthorhombic system.

All other magnetic lattices derived from \(F\) and \(I\) belong to the class \(P_S\) of the triclinic system.

Meaning of symbols used by Belov, Neronova and Smirnova.

Plain lattices \(P\).

\(P_S\) a primed translation along one edge,

\(P_a\) " " " " an edge in the \(a\) direction,

\(P_b\) " " " " an edge in the \(b\) direction,

\(P_c\) " " " " an edge in the \(c\) direction,

\(C_a\) " " " " edges in the \(a\) and \(b\) direction for the monoclinic and orthorhombic system,

\(P_C\) " " " " edges in the \(a\) and \(b\) directions for the tetragonal system,
$A_c$ a primed translation along edges in the $b$ and $c$ directions,

$I_c$ edges in the $a$, $b$ and $c$ directions in the tetragonal system,

$F_s$ edges in the $a$, $b$ and $c$ directions in the orthorhombic and cubic system,

Plain lattices $R$

$R_i$ a primed translation along edges in the $a$, $b$ and $c$ directions.

Base-centered lattices $C$

$C_c$ a primed translation along an edge in the $c$ direction,

$P_c$ the diagonals of the $C$ face,

$I_c$ the diagonals of the $C$ face and the edge in the $c$ direction in the orthorhombic system,

Face-centered lattices $F$

$C_A$ a primed translation along the diagonals of the $A$ and $B$ face,

$A_c$ the diagonals of the $B$ and $C$ face.

Body-centered lattices $I$

$P_i$ a primed translation along the body diagonal.
SECTION 4.3

In Section 2.1 we have given the definition \[(2.1.4)\] of a magnetic point group. There are 90 of such groups; 32 of them are the ordinary crystallographic point groups.

The properties of the magnetic point groups have been given implicitly in Chapter 2. Here we will only mention a property which is peculiar to magnetic point groups (or, more generally, peculiar to all magnetic rotation groups):

A rotation \(R_3\) of order 3 cannot be a primed element of a magnetic point group.

In fact if it was then \((R_3')^3 = E'\) would belong to the magnetic point group as well, which is not compatible with the definition of magnetic point group.

It should be mentioned that a rotation \(R_3\) never appears in the cosets of a point group \(\tilde{H}\) relative to its subgroups \(\tilde{H}^D\) so that the magnetic point groups are obtained by considering all the 32 ordinary point groups.

We now give a list of the 90 magnetic point groups, arranged into families; a "family" of magnetic point groups consists of a trivial magnetic point group \(H\) (that is, an "ordinary" point group) and of all magnetic point groups derived from \(\tilde{H}\) by means of rule 2.2.8. Each line in the list gives groups of one family.

The notation used in the list has been introduced by Belov, Neronova and Smirnova (1955), and is a straightforward generalization of the usual international notation for the
ordinary point groups. The international symbol for an ordinary point group indicates the generating elements of the group. In the symbol for a magnetic point group, those generating elements which are primed have a dash as a superscript. By omitting the dashes in the symbol of a magnetic point group, one obtains the symbol of the ordinary point group to whose family the magnetic point group in question belongs.

List of magnetic point groups

1

1

1' 1'

2

2 2'

m m'

2/m 2'm 2/m' 2'/m'

222 2'2'2

mm2 m'm2' m'm'2

mmm m'mm m'm'm m'm'm'

4 4'

4 4'

4/m 4'/m 4/m' 4'/m'

422 4'22' 42'2'

4mm 4'm'm 4m'm'
Our method of deriving all MSGs has a weakness which it shares with all systematic methods of deriving all ordinary space groups: it occasionally gives the same MSG more than
once. Here the phrase "the same MSG" is used in the following sense:

\[ \tilde{M}_1 \text{ and } \tilde{M}_2 \text{ are } \text{"the same" } = \tilde{M}_1 \text{ and } \tilde{M}_2 \text{ belong to the same } \text{"class of MSGs" } = \tilde{M}_1 \text{ and } \tilde{M}_2 \text{ are not } \text{"properly different" } = \tilde{M}_1 \text{ and } \tilde{M}_2 \text{ are } \text{"equivalent"}. \]

The definitions of the terms "properly different MSGs" and "a class of MSGs" have been given in Section 2.3.

In the present section we formulate a certain number of general theorems which enable us to decide whether or not two MSGs are equivalent. We do not give the proofs of these theorems because these proofs are all simple consequences of the basic properties of MSGs, and of the immediate implications of the definitions of such well-known concepts as isomorphism, automorphism, and equivalence of sets of matrices.

It will be convenient (but not necessary) to interpret, from now on, an MSG as a group of matrices of four columns and four rows as is often done in the case of ordinary space groups. Such an interpretation is possible because the one-to-one correspondence
is obviously an isomorphism (the 3x3-matrix R is the (proper or improper) rotation matrix, the $\tau_k$'s and $t_k$'s, $k = 1, 2, 3$, are components of $\tau$ and $t$ along the coordinate axes).

Using this interpretation the equivalence of two MSGs becomes simply the equivalence of two corresponding matrix groups, the equivalence transformation being a 4x4 matrix $S$ representing an element of the general inhomogeneous linear group $\tilde{C}$. More precisely:

(4.4.2) $\tilde{M}_1$ and $\tilde{M}_2$ are equivalent MSGs if and only if there exists a matrix $S$ such that $S\tilde{M}_1S^{-1} = \tilde{M}_2$.

Hence:

(4.4.3) If $\tilde{M}(\tilde{D}_1)$ and $\tilde{M}(\tilde{D}_2)$ are equivalent, then

$$S\tilde{D}_1S^{-1} = \tilde{D}_2$$
$$S(\tilde{M}(\tilde{D}_2) - \tilde{D}_1)S^{-1} = \tilde{M}(\tilde{D}_2) - \tilde{D}_2;$$
and the converse statement is also true

(4.4.4) If $\tilde{D}_1$ is a subgroup of index 2 of $\tilde{F}_1$ and $\tilde{D}_2$ is a subgroup of index 2 of $\tilde{F}_2$ then $\tilde{M}(\tilde{D}_1)$ and $\tilde{M}(\tilde{D}_2)$ are equivalent if and only if there exists a matrix $S$ such that

$$SD_1S^{-1} = \tilde{D}_2$$

$$S(F_1-\tilde{D}_1)S^{-1} = F_2-\tilde{D}_2.$$ 

From (4.4.4) we conclude:

(4.4.5) Two space groups from which two equivalent MSGs are derived are necessarily equivalent.

(4.4.6) Two equivalent MSGs necessarily belong to the same family.

(4.4.7) Two MSGs $\tilde{M}(\tilde{D}_1)$ and $\tilde{M}(\tilde{D}_2)$ are necessarily not equivalent if $\tilde{D}_1$ and $\tilde{D}_2$ are not equivalent.

A less trivial theorem also follows immediately from (4.4.4):

(4.4.8) If the subgroups $\tilde{D}_1$ and $\tilde{D}_2$ of two MSGs $\tilde{M}(\tilde{D}_1)$ and $\tilde{M}(\tilde{D}_2)$ derived from a space group $\tilde{F}$ are equivalent but the isomorphism implied by this equivalence is not induced by an automorphism of $\tilde{F}$, then $\tilde{M}(\tilde{D}_1)$ and $\tilde{M}(\tilde{D}_2)$ are not equivalent.

This automorphism of $\tilde{F}$ must be an outer automorphism as both $\tilde{D}_1$ and $\tilde{D}_2$ being invariant subgroups of $\tilde{F}$ are invariant under any inner automorphism of $\tilde{F}$.

However:
(4.4.9) If the subgroups \( \tilde{D}_1 \) and \( \tilde{D}_2 \) of two MSGs \( \tilde{M}(\tilde{D}_1) \) and \( \tilde{M}(\tilde{D}_2) \) derived from a space group \( \tilde{F} \) are equivalent and the isomorphism implied by this equivalence is induced by an automorphism of \( \tilde{F} \), \( \tilde{M}(\tilde{D}_1) \) and \( \tilde{M}(\tilde{D}_2) \) need not be equivalent. (To decide whether they are equivalent or not one has to compare the traces of all matrices \( \tilde{M}(\tilde{D}_1) \) and \( \tilde{M}(\tilde{D}_2) \) which correspond to one another under the isomorphism between \( \tilde{M}(\tilde{D}_1) \) and \( \tilde{M}(\tilde{D}_2) \) induced by the automorphism of \( \tilde{F} \).)

We shall now give a certain number of rules concerning the equivalence of the subgroups \( \tilde{D} \) of a space group \( \tilde{F} \) and the equivalence of the MSGs derived from them.

(4.4.10) A subgroup \( \tilde{D}_T \) of a given space group \( \tilde{F} \) can never be equivalent to a subgroup \( \tilde{D}_R \) of \( \tilde{F} \).

(4.4.11) An MSG \( \tilde{M}(\tilde{D}_T) \) and an MSG \( \tilde{M}(\tilde{D}_R) \) derived from a space group \( \tilde{F} \) are never equivalent.

(4.4.12) Two subgroups \( \tilde{D}_T \) of a space group \( \tilde{F} \) may be equivalent or not. If they are not equivalent the corresponding MSGs are necessarily not equivalent. If they are equivalent the corresponding MSGs may still be equivalent or not.

(4.4.13) Let \( \tilde{D}_{T1} \) and \( \tilde{D}_{T2} \) be two subgroups of \( \tilde{F} \) and let \( \tilde{R}^{D}_{1} \) and \( \tilde{R}^{D}_{2} \) be their point groups. If \( \tilde{R}^{D}_{1} \) and \( \tilde{R}^{D}_{2} \) are not isomorphic, then \( \tilde{D}_{T1} \) and \( \tilde{D}_{T2} \) are necessarily not equivalent and hence \( \tilde{M}(\tilde{D}_{T1}) \) and \( \tilde{M}(\tilde{D}_{T2}) \) are not equivalent either. If \( \tilde{R}^{D}_{1} \) and \( \tilde{R}^{D}_{2} \) are isomorphic and equivalent then
\( \mathcal{T}_1 \) and \( \mathcal{T}_2 \) are equivalent only if the 3x3 matrix which transforms \( \mathcal{R}_1 \) into \( \mathcal{R}_2 \) transforms the lattice \( \mathcal{T} \) into a lattice of the same class to which \( \mathcal{T} \) belongs and the non-primitive translation of every element of \( \mathcal{R}_1 \) into the non-primitive translation of its corresponding element in \( \mathcal{R}_2 \). The isomorphism between \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \) implied by their equivalence is then induced by an automorphism of \( \mathcal{F} \), and the MSGs \( \tilde{\mathcal{M}}(\mathcal{T}_1) \) and \( \tilde{\mathcal{M}}(\mathcal{T}_2) \) may but need not be equivalent (compare 4.4.9).

(4.4.14) The subgroups \( \mathcal{D}_R \) and \( \mathcal{D}_a \) of a space group \( \mathcal{F} \) derived from a subgroup \( \mathcal{Q} \) or \( \mathcal{Q}_r \) of index 4 of \( \mathcal{F} \) are equivalent if the translation \( t \) which appears in some elements of \( \mathcal{D}_a \) can be transformed away from all of them.

In fact \( \mathcal{D}_R \) and \( \mathcal{D}_a \) have the same point group and the same lattice and if the equivalence transformation \( S \) such that \( \mathcal{D}_R = S \mathcal{D}_a S^{-1} \) exists it is a pure translation and hence leaves the point group and the lattice of \( \mathcal{D}_a \) unchanged.

(4.4.15) Two MSGs \( \tilde{\mathcal{M}}(\mathcal{D}_R) \) and \( \tilde{\mathcal{M}}(\mathcal{D}_a) \) derived from a space group \( \mathcal{F} \) are equivalent if \( \mathcal{D}_R \) and \( \mathcal{D}_a \) are equivalent. In this case the equivalence of \( \mathcal{D}_R \) and \( \mathcal{D}_a \) is a sufficient condition for the equivalence of \( \tilde{\mathcal{M}}(\mathcal{D}_R) \) and \( \tilde{\mathcal{M}}(\mathcal{D}_a) \).

(4.4.16) Two subgroups \( \mathcal{D}_R \) and \( \mathcal{D}_a \) of a space group \( \mathcal{F} \) are equivalent if their lattices \( \mathcal{T}_1 \) and \( \mathcal{T}_2 \) belong to the same Bravais class and if the matrix which transforms
\[ \mathcal{T}_1 \] into \[ \mathcal{T}_2 \] leaves the non-primitive translations (if any) of the elements of the point group \( \mathcal{H} \) unchanged.

(4.4.17) If the isomorphism implied by the equivalence of two subgroups \( \mathcal{D}_{R_{Q1}} \) and \( \mathcal{D}_{R_{Q2}} \) or \( \mathcal{D}_{R_{\alpha 1}} \) and \( \mathcal{D}_{R_{\alpha 2}} \) of a space group \( \mathcal{F} \) is induced by an automorphism of \( \mathcal{F} \), then the two corresponding MSGs may but need not be equivalent.

(4.4.18) A subgroup \( \mathcal{D}_{R_{\alpha}} \) and a subgroup \( \mathcal{D}_{R_{\gamma}} \) of a space group \( \mathcal{F} \) derived from two different subgroups \( \mathcal{Q}_{\gamma} \) of index 4 of \( \mathcal{F} \) can be equivalent only if the translation \( t_{\alpha} \) can be transformed away from \( \mathcal{D}_{R_{\alpha}} \), if the lattices of the two space groups belong to the same Bravais class and if the matrix which transforms one of the two lattices into the other transforms the non-primitive translation of an element of the first group into the non-primitive translation of the corresponding element in the second group. Again the isomorphism between the two groups may or may not be induced by an automorphism of \( \mathcal{F} \) and hence the two corresponding MSGs may or may not be equivalent.

SECTION 4.5

In Section 3.4 we have derived all the subgroups of index 2 of the space groups \( P4 \), \( P4_1 \), \( P4_2 \) and \( P4_3 \). We will now give the corresponding MSGs arranged into families.

As we have said in Section 3.4 the space group \( P4 \) has only one subgroup \( \mathcal{D}_{T} \). To this subgroup there corresponds the
MSG $P_4^\prime$ which consists of the elements

$$(E|n_1a+n_2b+n_3c),(C_{4|x}|0),(C_{4|x}|0),(C_{4|x}|0),\frac{1}{2}(E|c)')$$

To the subgroup $\tilde{D}_{Rq}$ of $P_4$ which is obtained from $\tilde{Q}_1$ (See Section 3.4) there corresponds the MSG $P_{c4}$ which consists of the elements

$$(E|n_1a+n_2b+2n_3c),(C_{4|x}|0),(C_{4|x}|0),(C_{4|x}|0),(E|c)',\frac{1}{2}(E|c)')$$

To the subgroup $\tilde{D}_{Rq}$ of $P_4$ which is obtained from the same $\tilde{Q}_1$ there corresponds the MSG $P_{c4}2$ which consists of the elements

$$(E|n_1a+n_2b+2n_3c),(C_{4|x}|c),(C_{4|x}|0),(C_{4|x}|0),(E|c),\frac{1}{2}(E|c))$$

Obviously $P_{c4}$ and $P_{c4}2$ are not equivalent.

To the subgroups $\tilde{D}_{Rq}$ and $\tilde{D}_{Rq}$ of $P_4$ which are equivalent and obtained from $\tilde{Q}_2$ there corresponds one MSG $P_{c4}$ which consists of the elements

$$(E|2n_1a+n_2(a+b)+n_3c),(C_{4|x}|0),(C_{4|x}|0),(C_{4|x}|0),(E|c),\frac{1}{2}(E|c)')$$

To the subgroups $\tilde{D}_{Rq}$ and $\tilde{D}_{Rq}$ of $P_4$ which are equivalent and obtained from $\tilde{Q}_3$ there corresponds one MSG $I_{c4}$ consisting of the elements

$$(E|2n_1a+n_2(a+b)+n_3(a+c),(C_{4|x}|0),(C_{4|x}|0),(C_{4|x}|0),(E|c',\frac{1}{2}(E|c)')$$
Thus the family \(P_4\) consists of \(P_4, P_4', P_{4c}, P_{4c2}, P_{4c4}, I_{4c}\).

The space group \(P_{41}\) has only one subgroup \(\tilde{D}_T\) to which there corresponds the MSG \(P_{41}'\). This group consists of the elements

\[
(E|n, a + n_1b + n_2c), (C_{4z} \frac{1}{2}), (C_{4z} \frac{c}{2}), (C_{4z} \frac{3c}{2})
\]

The group \(P_{41}\) has also only one subgroup \(\tilde{D}_{R_{01}}\) and \(\tilde{D}_{R_{02}}\). They are equivalent and to them there corresponds one MSG \(P_{4c41}\) which consists of

\[
(E|2n, a + n_1b + n_2c), (C_{4z} \frac{1}{2}), (C_{4z} \frac{c}{2}), (C_{4z} \frac{3c}{2}), (E|a)
\]

Thus the family of \(P_{41}\) consists of \(P_{41}, P_{41}', P_{4c41}\).

Similarly, from the space group \(P_{42}\) the following MSGs are derived:

\(P_{42}'\) which consists of the elements

\[
(E|n, a + n_1b + n_2c), (C_{4z} \frac{1}{2}), (C_{4z} \frac{c}{2}), (C_{4z} \frac{3c}{2})
\]

\(P_{4c41}\) which consists of the elements

\[
(E|n, a + n_1b + 2n_2c), (C_{4z} \frac{c}{2}), (C_{4z} \frac{c}{2}), (C_{4z} \frac{3c}{2}), (E|c)
\]
\[ P_{C43} \] which consists of the elements
\[ (E|n_1a + n_1b + 2n_3c), (C_{4z}| \frac{c}{2} + c), (C_{4z}| \frac{3c}{4}) \]

\[ P_{C42} \] which consists of the elements
\[ (E|2n_1a + n_2(a+b) + n_3c), (C_{4z}| \frac{c}{2}), (C_{4z}| \frac{3c}{4}), (E|\alpha) \]

\[ I_{C41} \] which consists of the elements
\[ (E|2n_1a + n_2(a+b) + n_3(a+c)), (C_{4z}| \frac{c}{2}), (C_{4z}| \frac{3c}{4}), (E|\alpha) \]

Thus the family of \( P_{42} \) consists of \( P_{42}, P_{42}', P_{C41}, P_{C43}, P_{C42}, I_{C41} \).

From the space group \( P_{43} \) the following MSGs are derived:

\[ P_{43}' \] which consists of the elements
\[ (E|n_1a + n_1b + n_2c), (C_{4z}| \frac{c}{2}), (C_{4z}| \frac{3c}{4}) \]

\[ P_{C43} \] which consists of the elements
\[ (E|2n_1a + n_2(a+b) + n_2c), (C_{4z}| \frac{3c}{4}), (C_{4z}| \frac{3c}{4}), (E|\alpha) \]

Thus the family of \( P_{43} \) consists of \( P_{43}, P_{43}', P_{C43} \).
NOTES TO CHAPTER 4.

Graphical representation of all black-and-white lattices (magnetic lattices) can be found in a paper by Belov, Neronova and Smirnova (1955), and in a review article by Le Corre (1959).

A list in which all black-and-white lattices seem to be arranged into families is given by Zamorzaev (1957). The uncertainty arises from the lack of any comments on the part of the author, and from some minor inconsistencies which may be due to misprints.

Magnetic point groups were first listed by Heesch (1929) and more recently again by Tavger and Zaitsev (1956) who do not quote Heesch. A list in which magnetic point groups are arranged into families is given by Le Corre (1959).

Finally it should be mentioned that there exists an entirely different method to derive all MSGs. It is a special case of a very general method recently proposed by Bienenstock and Ewald (1962) to investigate systematically the symmetries of the reciprocal or Fourier space of a crystal.
CHAPTER 5

INVARIANT ARRANGEMENTS OF SPINS

In Section 5.1 we consider MSGs in their relation to the invariant arrangements of (average) magnetic moments in ferromagnetic, ferrimagnetic and antiferromagnetic crystals. In Section 5.2 we describe a procedure for determining the MSG which leaves invariant a given arrangement of magnetic moments.

For simplicity, we will call an arrangement of magnetic moments an "arrangement of spins", that is, the average magnetic moment of an individual magnetic atom will be simply called a "spin".

While in Chapters 2, 3 and 4 the physical meaning attached to the element $E'$ of $\tilde{\Lambda}$ could be left unspecified, in the present chapter it becomes essential to interpret $E'$ as time-reversal.

SECTION 5.1

We begin with stating explicitly the well-known transformation properties of the spin (they were already used in introducing the definition of MSGs in Chapter 1):

(5.1.1) For proper and improper rotations the spin is an axial vector, for time-reversal it is a polar vector; the only effect of time-reversal on the spin is to change its "sense", the "direction" of the spin remaining the same.
Some simple rules follow immediately from 5.1.1:

(5.1.2) A spin of a given direction and sense is transformed into another spin of the same direction and sense under any translation, under a proper or improper rotation about an axis parallel to the spin (hence under a reflection in a plane perpendicular to the direction of the spin) and under space inversion.

(5.1.3) If a spin is along an axis of proper rotations, or its origin is in a reflection plane perpendicular to the spin or at a center of inversion, it is left invariant under the proper rotation, the reflection or the space inversion respectively. If a spin is along an axis of an improper rotation but its origin is not at the center of inversion, then it is transformed by the improper rotation into another spin of the same direction and sense.

(5.1.4) A spin of a given direction and sense is transformed into another spin of the same direction and opposite sense by a proper or improper rotation through 180° about an axis perpendicular to the direction of the spin.

(5.1.5) A spin is transformed into another spin of the same direction but opposite sense under a primed translation, under a primed proper or improper rotation about an axis parallel to the spin and finally under the combination of space inversion with time-reversal (primed space inversion) when the origin of the given spin is not at the center of inversion. (This follows from (5.1.1) and (5.1.2)).
(5.1.6) No spin can be along an axis of a primed proper rotation, can have its origin at a center of a primed space inversion or can be perpendicular to a plane of primed reflection and have its origin on the plane. These restrictions arise from the fact that no two spins of opposite sense can be at the same point in the crystal. Thus they do not hold any longer if the primed proper rotation, the primed space inversion and the primed reflection mentioned above are followed by non-primitive translations.

(5.1.7) A spin of a certain direction and sense is transformed into another spin of the same direction and sense under a primed proper or improper rotation of order \(2\) about an axis perpendicular to the direction of the spin. (This follows from (5.1.1) and (5.1.4)).

(5.1.8) In particular, if a spin has its origin on an axis of a primed proper or improper rotation of order \(2\) it is left invariant under the rotation.

An illuminating graphical representation of the above rules has been given by Donnay, Corliss, Donnay, Elliott and Hastings (1958) in Fig. 1 of their paper.

An essential part of the contents of rules (5.1.2) - (5.1.8) can be formulated as follows:

(5.1.9) The direction and sense of a spin are left invariant under the group \(\bar{\alpha} \frac{1}{m} \frac{1}{m'} \frac{1}{m'}\) and hence under any of its subgroups. Here \(\bar{\alpha} \frac{1}{m} \frac{1}{m} \frac{1}{m} \) stands for any rotation about an axis parallel to the direction of the spin, \(\frac{1}{m} \frac{1}{1} \frac{1}{1}\) stands
for a reflection in a plane perpendicular to the direction of the spin, \( \frac{1}{1} \frac{2'}{1} \frac{1}{1} \) and \( \frac{1}{1} \frac{1}{1} \frac{2'}{1} \) for two primed rotations of order 2 about two axes perpendicular to the direction of the spin and to each other respectively, \( \frac{1}{1} \frac{1}{1} \frac{1}{1} \) and \( \frac{1}{1} \frac{1}{1} \frac{1}{1} \) for primed reflections in two planes perpendicular to the two previously defined axes.

Consider now a magnetic crystal both as an arrangement of spins and an arrangement of atoms.

(5.1.10) We shall say that a magnetic crystal is invariant under an MSG \( \tilde{M} \) if it is indistinguishable both as an arrangement of atoms and an arrangement of spins from the crystal obtained from it by applying all unprimed and primed elements of \( \tilde{M} \).

(5.1.11) If a magnetic crystal as an arrangement of atoms is invariant under a space group \( \tilde{F} \), then, as an arrangement of spins, it is either invariant under an MSG of the family of \( \tilde{F} \), in particular under \( \tilde{F} \) itself, or under a member of the family of a subgroup of \( \tilde{F} \).

(5.1.12) Conversely, if a magnetic crystal as an arrangement of spins is invariant under an MSG \( \tilde{M} \) it is invariant, as arrangement of atoms, under the space group \( \tilde{F} \) to whose family \( \tilde{M} \) belongs. (The statement is trivial if \( \tilde{M} \) coincides with \( \tilde{F} \), and is easily proved in other cases if one remembers the way in which an MSG \( \tilde{M}(\tilde{F}) \) is derived from a space group \( \tilde{F} \)).

We are now in a position to discuss the MSGs in
their relation to magnetic crystals. First of all we shall distinguish between MSGs which can leave ferromagnetic crystals invariant and MSGs which cannot. We shall call them "ferromagnetic" and "non-ferromagnetic" space groups respectively. More precisely:

(5.1.13) We shall say that an MSG $\tilde{M}$ is "ferromagnetic" if there exists at least one direction such that a spin arrangement in which all the spins have that direction and a given sense is invariant under all primed and unprimed elements of $\tilde{M}$.

As ferromagnetic crystals have a non-zero macroscopic magnetic moment in some well-defined direction, the magnetic point group belonging to an MSG $\tilde{M}$ which leaves a ferromagnetic crystal invariant has to be, according to (5.1.9), a subgroup of $\frac{\infty}{m}, \frac{2l}{m}, \frac{2l}{m}$. There are 31 of such subgroups and their list is given at the end of this section. There we also indicate the direction that a spin must have to be transformed into a spin of the same direction and sense under each of the 31 subgroups of $\frac{\infty}{m}, \frac{2l}{m}, \frac{2l}{m}$.

Obviously the translations of an MSG $\tilde{M}$ which leaves a ferromagnetic crystal invariant must be ordinary translations, and hence $\tilde{M}$ is either an ordinary space group or an MSG of the kind $\tilde{M}_T$.

Hence:

(5.1.14) An MSG $\tilde{M}$ is ferromagnetic if and only if its point group is a subgroup of $\frac{\infty}{m}, \frac{2l}{m}, \frac{2l}{m}$, and if it is either an ordinary space group or of the kind $\tilde{M}_T$. 
There are 275 ferromagnetic space groups. They are marked with an asterisk in the list of MSGs at the end of this thesis.

We have considered so far only ferromagnetic spin arrangements. We want now to make a few remarks about ferrimagnetic and antiferromagnetic spin arrangements. All these remarks are essentially based on the fact that according to (5.1.3) the spins can only occupy those sites in a crystal whose symmetry groups are subgroups of

\[ \infty \, \frac{2'}{m'} \, \frac{2'}{m'} \cdot \]

Invariant ferrimagnetic spin arrangements are of course compatible with ferromagnetic space groups only. And, conversely, for each of the 275 ferromagnetic space groups there exists an invariant ferrimagnetic spin arrangement. However, in view of (5.1.14), these ferrimagnetic arrangements cannot be of a collinear type if there is only one spin per unit cell. In order to have collinear type of ferrimagnetic arrangements there must be at least two spins per unit cell.

In a non-collinear ferrimagnetic crystal spins cannot occupy positions whose symmetry group is different from \(1, \bar{1}, 2', m', 2'/m', 2'm'm'\). In fact, if the symmetry of a site where a spin is situated is a subgroup of \(\infty \, \frac{2'}{m'} \, \frac{2'}{m'} \)

different from the groups just enumerated, the spin can only be in one fixed direction which is left unchanged by the magnetic point group of the ferromagnetic space group being considered.
In particular if the point group belonging to the space group of a crystal contains rotations of order higher than 2, spins cannot occupy sites whose symmetry groups contain elements of order higher than 2. It seems that atoms are preferentially situated at sites of higher symmetry in a crystal, it follows that the ferromagnetic space group which leaves a non-collinear ferrimagnetic crystal invariant cannot contain elements of order higher than 2.

Every MSG leaves some antiferromagnetic arrangements of spins invariant. If an MSG is of the kind \( \tilde{M}_T \) but not ferromagnetic then an antiferromagnetic spin arrangement left invariant by it must be non-collinear.

Turning now to the MSGs of the kind \( \tilde{M}_R \), we have to distinguish here between those MSGs \( \tilde{M}_R \) whose point group is a subgroup of \( \frac{\infty}{m} \frac{2'}{m'} \frac{2'}{m'} \) with no primed elements, and the remaining MSGs \( \tilde{M}_R \). In the former case only collinear antiferromagnetic spin arrangements are possible; in the latter case only non-collinear ones. These statements presuppose that there is only one spin per unit cell or, more precisely, that the whole spin arrangement can be obtained by applying all the operations of the MSG to a single spin.
List of the 31 subgroups of $\infty \overset{2'}{m} \overset{2'}{m}$

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SECTION 5.2

In this section we make some general remarks concerning the determination of the MSGs of a magnetic crystal assuming that its structure and the arrangement of its spins are known.

As has already been stated, the symmetry of the sites occupied by magnetic atoms must be such that a spin located in any of those sites is left unchanged by the elements of the symmetry groups of the sites. Hence, as we have seen before, the symmetry groups of the sites occupied by magnetic atoms must be subgroups of \( \tilde{\Sigma} \frac{2'}{m} \frac{2'}{m'} \).

It follows that if the magnetic atoms of a crystal invariant under a space group \( \tilde{\mathcal{F}} \) occupy sites whose symmetry groups are point groups whose families contain subgroups of \( \frac{\infty}{m} \frac{2'}{m} \frac{2'}{m'} \), the MSG which leaves the magnetic crystal
invariant may belong to the family of $\tilde{F}$; in the opposite case it must necessarily belong to the family of a subgroup of $\tilde{F}$. In order to accommodate the magnetic atoms in their sites, this subgroup of $\tilde{F}$ must have some special sites in common with $\tilde{F}$, and these sites must have symmetry groups which satisfy again the conditions just formulated. This subgroup of $\tilde{F}$ may or may not belong to the same system as $\tilde{F}$. If it does then the magnetic and the ordinary lattice must have the same holohedry. If it does not then the two lattices have different holohedry.

Consider, for example, a crystal whose space group belongs to the cubic system. Suppose it is ferromagnetic. There are no ferromagnetic space groups belonging to the cubic system. Thus the MSG of the crystal must belong either to the rhombohedral, tetragonal, orthorhombic, monoclinic or triclinic system and the magnetic lattice does not belong to the cubic system.

Similar considerations apply to the case of ferrimagnetic and antiferromagnetic crystals.

In particular, in the case of antiferromagnetic crystals it is possible to exclude many MSGs as incompatible with a given arrangement of spins on the basis of general relationships between spin arrangements and MSGs described at the end of Section 5.1.
As an example of what has been said in this chapter we shall briefly discuss the magnetic structure of MnO.

MnO is an antiferromagnetic crystal. We assume that its space group is Fm3m, (there is some doubt about the correctness of this assumption). The Mn atoms are in the sites

\[ m3m \quad 000, \frac{1}{2} \frac{1}{2} 0, \frac{1}{2} 0 \frac{1}{2}, 0 \frac{1}{2} \frac{1}{2} \]

The group m3m is not a subgroup of \( \frac{1}{2} \frac{1}{2} \frac{1}{2} \), nor does any such subgroup belong to the family of m3m. It follows that the MSG of the crystal must belong to the family of a subgroup of Fm3m.

The lattice of Fm3m is a face-centered cubic lattice, thus the non-primitive parallelepiped unit cell of the crystal is a cube. From neutron diffraction experiments it is known that parallel spins lie in (111)-planes of the cubic lattice, and that spins lying in two consecutive (111)-planes are antiparallel; however the direction of the spins in the planes is not known.

As the magnetic unit cell of MnO one usually takes a cube whose volume is eight times that of the cubic unit cell defined above. If \( \ell \) is the edge of the parallelepiped unit cell of Fm3m, \( 2 \ell \) is the edge of the magnetic parallelepiped unit cell. One can easily convince oneself that this arrangement of spins is compatible with the magnetic lattice \( C_C \) of the monoclinic system; the C face being parallel to the (111)-plane and the c-axis being along the diagonal [110].
In the new lattice $C$ the magnetic atoms are at

$$000, 00\frac{4}{2}, \frac{4}{2} \frac{4}{2} 0, \frac{4}{2} \frac{4}{2} \frac{4}{2}$$

There are two MSGs with lattice $C_C$ and the four positions just listed. They are $C_C2/m$ and $C_C2/c$.

If $a, b, c$ are the three edges of the parallelepiped unit cell of $C$, $C_C2/m$ consists of

$$(E| \frac{m_1 a + b}{2} + m_2 b + 2m_3 c), (C_{2y}|0), (I|0), (E|C)'$$

whereas $C_C2/c$ consists of

$$(E| m_1 a + b + m_2 b + 2m_3 c), (C_{2y}|c), (I|0), (\sigma_x|c), (E|c)'$$

In $C_C2/m$ the symmetry group of the sites of the Mn atoms is $2/m$, in $C_C2/c$ it is $2'/m'$. It follows that if spins in the (111)-plane are parallel to the $b$-direction the MSG is $C_C2/m$. If spins are parallel to the $a$-direction then the MSG is $C_C2/c$. Should spins be in neither of these directions the MSG would be $P_{\bar{1}}$, that is, an MSG of the triclinic system.

NOTES TO CHAPTER 5

The list of the 31 subgroups of $\begin{array}{c} 2'/m' \\ m \\ m' \end{array}$ was first given by Tavger (1958).

The list of the 275 ferromagnetic groups was first given by Neronova and Belov (1960).
LIST OF SYMBOLS

$\mathcal{C}$ general inhomogeneous linear group

$\tilde{F}$ space group, or class of equivalent space groups

$\tilde{A}$ abstract group of two elements $E$ (identity) and $E'$; also the time-reversal group.

$\tilde{D}^H$ subgroup of index 2 (due) of the group $\tilde{H}$

$\tilde{D} = \tilde{D}^F$ subgroup of index 2 of a space group $\tilde{F}$

$\tilde{D}_T$ $\tilde{D}^F$ which has the same lattice $\tilde{T}$ as $\tilde{F}$

$\tilde{D}_R$ $\tilde{D}^F$ which has the same point group $\tilde{R}$ as $\tilde{F}$

$\tilde{D}_{Ro}$ and $\tilde{D}_{Ra}$ two kinds of $\tilde{D}_R$

$\tilde{T}$ lattice (that is, group of primitive translations)

$\tilde{T}^D = \tilde{T}^D$ point group

$\tilde{R}^D = \tilde{D}_R$

$\tilde{Q}$ subgroup of index 4 (quattro) of a symmorphic $\tilde{F}$

$\tilde{Q}_\tau$ subgroup of index 4 of a non-symmorphic $\tilde{F}$

$\tilde{Q}_{\tau_0}$ and $\tilde{Q}_{\tau_\alpha}$ two kinds of $\tilde{Q}_\tau$

$\tilde{M}$ magnetic space group, or class of magnetic space groups

$\tilde{M}(\tilde{D})$ magnetic space group whose unprimed elements form the group $\tilde{D}$

$\tilde{M}_T = \tilde{M}(\tilde{D}_T)$

$\tilde{M}_R = \tilde{M}(\tilde{D}_R)$

$\tilde{M}_{Ro} = \tilde{M}(\tilde{D}_{Ro})$

$\tilde{M}_{Ra} = \tilde{M}(\tilde{D}_{Ra})$

$\tilde{T}_M$ magnetic lattice of $\tilde{M}$

$\tilde{R}_M$ magnetic point group of $\tilde{M}$
LIST OF MAGNETIC SPACE GROUPS

(MSGs of the orthorhombic system are not included.)

Notation and arrangement are explained in Chapter 4.

Triclinic system

- $C_{a\bar{2}}$  $P_{a\bar{m}}$
- $P_{b\bar{2}1}$  $P_{b\bar{m}}$

1

- $*P_{1}$  $C_{a\bar{m}}$
- $P_{s\bar{1}}$  $*P_{2\bar{1}}$  $P_{c\bar{c}}$
- $*P_{2'\bar{1}}$

$\bar{1}$

- $P_{a2\bar{1}}$  $*P_{c\bar{c}}$
- $*P_{1\bar{1}}$  $*P_{c'}$
- $P_{1'\bar{1}}$  $*C_{2}$  $P_{a\bar{c}}$
- $P_{s\bar{1}}$  $*C_{2'}$  $P_{b\bar{c}}$
- $C_{c\bar{2}}$

Monoclinic system $P_{c\bar{2}}$

2

- $P_{C2\bar{1}}$  $*C_{m}$
- $*P_{2}$  $*C_{m'}$
- $*P_{2'}$  $*P_{m}$  $C_{c\bar{m}}$
- $P_{a\bar{2}}$  $*P_{m'}$
- $P_{b\bar{2}}$  $P_{c\bar{m}}$
- $P_{A\bar{c}}$
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2/m

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Note: The table represents crystallographic information, where each row lists a specific crystal structure and its corresponding space group and symmetry.
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R3m  *P6₁  6/m

R3' m  P6₁  *P6/m

R3 ' m'  P6/m'

*R3m'  *P6₅

R₁3m  P6₅'

R₁3c  *P6₂  P₆₂/m

R3c  P₆₂  *P6₃/m

R₃c'  P₆₅₁  *P6²₂

R₃ ' c'  P₆₅₄  P₆₅₂/m

*R₃c'  *P6₄

P₆₄'

Hexagonal system

Pc₆₂  622

6  Pc₆₂₂  *P6

P₆'

P₆²²

Pc₆  *P6

P₆₂  *P6²₂

Pc₆₃  *P6'

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P_6\overline{3}/m'm'c & \quad P_{I\text{m}3} \\
P_6\overline{3}/m'm'c' & \quad \\P_6\overline{3}/m'mc' & \quad \text{Pa}3 \\
Pm3 & \quad \text{Pa}'3 \\
Pm'3 & \quad \\F_{s\text{m}3} & \quad \text{Ia}3 \\
\text{Cubic} & \quad \text{Pn3} \\
\text{system} & \quad \text{Pn}\text{3} \\
\text{P}_23 & \quad F_{s\text{d}3} \\
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P23 & \quad P_{432} \\
F_{s23} & \quad P_{4'32'} \\
F23 & \quad F_{\text{m}'3} \\
F_{s432} & \quad \\I23 & \quad F_{\text{d}3} \\
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