REPRESENTATIONS OF THE SPACE GROUP D_{4h}^{19},

AND THE CORRESPONDING DOUBLE SPACE GROUP

by

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ABSTRACT

One of the existing methods of calculating the characters of irreducible representations of space groups and double space groups is described in some detail, and applied to the case of the non-symmorphic space group D_{4h}^{19} ($I4_1/amd$) (which is the space group of crystals of white tin).

A complete list of the characters of irreducible representations of this space group and the corresponding double group is given. Some useful relations involving the characters are also included.

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CHAPTER I

Introduction

It is a well known fact that representations of space groups play an essential part in the theoretical description of many solid state phenomena. The theory of lattice vibrations, and that of electron band structure are probably the two most important examples of this fact. In the latter case the existence of the electronic spin necessitates dealing with the representations of double space groups in addition to those of space groups.

Although the general theory of the irreducible representations of space groups was given by Seitz (1936) more than twenty years ago, and the characters for the space groups O_h^1, O_h^9 and O_h^5 (single, body-centered and face-centered cubic lattices) were calculated soon after by Bouckaert, Smoluchowski and Wigner (1936), there are many non-trivial space groups for which this has not yet been done.

The work on irreducible representations of double space groups was started only a few years ago, by Elliott (1954).

The list of space groups for which the characters of irreducible representations have been calculated and published is given in the following table:

Space Group	Typical Crystal Structure	Reference
O_h^1 (Pm3m)	Simple cubic	L. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. 50, 58 (1936). (D)* R.J. Elliott, Phys. Rev. 96, 280 (1954).
O_h^5 (Fm3m)	Face-centered cubic	Bouckaert, Smoluchowski and Wigner, ibid. (D) Elliott, ibid.
O_h^7 (Fd3m)	Diamond	C. Herring, J. Franklin Inst. 233, 525 (1942). W. Döring and V. Zehler, Ann. Physik 13, 214 (1953). (D) Elliott, ibid.
O_h^9 (Im3m)	Body-centered cubic	Bouckaert, Smoluchowski and Wigner, ibid. (D) Elliott, ibid.
T_d^2 (F$\bar{4}$3m)	Zincblende	R.H. Parmenter, Phys. Rev. 100, 573 (1955). G. Dresselhaus, Phys. Rev. 100, 580 (1955). (D) Parmenter, ibid. (D) Dresselhaus, ibid.
D_{6h}^4 ($P6_3$/mmc)	Hexagonal close packed	Herring, ibid. (D) Elliott, ibid.
D_3^6 ($P3_221$)	Tellurium	Yu.A. Firsov, J. Exptl. Theoret. Phys. (USSR) 32, 1350 (1957). (D) Firsov, ibid.
C_{6v}^4 (C6mc)	Graphite	J.L. Carter, Ph.D. Thesis, Cornell University, February 1953 (unpublished). (D) J.C. Slonczewski, Ph.D. Thesis, Rutgers University, June 1955 (unpublished).
	Wurzite	R.C. Casella, Phys. Rev. 114, 1514 (1959). (D) Casella, ibid.

Space Group	Typical Crystal Structure	Reference
		G. Dresselhaus, Phys. Rev. 105, 135 (1957). (D) Dresselhaus, ibid.

* (D) means that the characters of the double space group are given in the reference in question.

In this thesis we outline a method, first used by Herring (1942) of calculating the characters of the irreducible representations of a space group, and apply it to the case of the space group D_{4h}^{19} (in which white tin crystalizes). We also adapt the method to the case of double space groups, and apply it to the double space group $D_{4h}^{19\,\dagger}$.

We shall now turn to a brief summary of the contents of the remaining chapters.

In the first part of Chapter II we introduce the concept of space group and discuss some properties of space groups. In the last part we discuss the space group D_{4h}^{19}.

In the first part of Chapter III, after having introduced the irreducible representations of a lattice, we define the concept of the Brillouin zone (B-Z). We then give the definition of the group G^k of a vector k and outline the method of finding its irreducible representations when k ends inside or on the surface of the B-Z. The concepts of the kernel T^k of a representation and factor group G^k/T^k are introduced. Finally we outline the method to construct an irreducible representation of a space group G from a given irreducible representation of a group G^k. In the remaining part of the chapter we apply the theory previously described to the case of D_{4h}^{19}. We examine the groups G^k of vectors k inside and on the surface of the B-Z of D_{4h}^{19} and we give their tables of characters. We also consider points on lines of symmetry in order to give the so called "compatibility relations" for the group in question.

In Chapter IV we introduce the concept of double space group and discuss its properties, and we construct the tables of characters of the double space group $D_{4h}^{19\,\dagger}$.

Some compatibility tables are included.

CHAPTER II

Space Groups and Their Properties

Discussion of a Special Case (Space Group D_{4h}^{19}, White Tin)

II.1 Let us consider the linear inhomogeneous transformations of the form:

$$\vec{r}' = R\vec{r} + \vec{t} \qquad \text{II.1.1}$$

where $\vec{r}$ and $\vec{r}'$ are position vectors of a point, R is a real orthogonal three-dimensional matrix and $\vec{t}$ is a real three-dimensional vector. The real orthogonal matrix R can be interpreted as either a proper or improper rotation according as det(R) is +1 or -1 respectively. Improper rotations are the inversion and operations representing a rotation followed by an inversion. The vector $\vec{t}$ can be interpreted as a translation, so that the transformation II.1.1 can be looked upon as a proper or improper rotation R followed by a translation $\vec{t}$. Using Seitz' symbolism we will denote the transformation II.1.1 by $(R|t)$.

The product of two inhomogeneous transformations is given by:

$$(R|t)(S|t') = (RS|Rt' + t) \qquad \text{II.1.2}$$

The inverse of a transformation (R | t) is:

$$(R|t)^{-1} = (R^{-1}|-R^{-1}t) , \qquad \text{II.1.3}$$

and the conjugate of (R|t) is:

$$(S|t')^{-1}(R|t)(S|t') = (S^{-1}RS|S^{-1}Rt' + S^{-1}t - S^{-1}t') \qquad \text{II.1.4}$$

From the definition of the multiplication II.1.2, of the inverse of an element II.1.3 and from the existence of the identity (E | 0) it follows that the set $\mathcal{R}$ of all real nonsingular inhomogeneous transformations (R | t) is a group.

A subgroup R_3 of $\mathcal{R}$ is the set of all "pure" rotations (R | 0). Such subgroup is the group R_3 of all the three-dimensional orthogonal matrices. Another subgroup of $\mathcal{R}$ is the set of all "pure" translations (E | t) in the group. Such subgroup is an invariant subgroup of $\mathcal{R}$. A crystallographic space group G is a special kind of subgroup of $\mathcal{R}$. A crystallographic space group G is in fact a discrete subgroup of $\mathcal{R}$ such that its pure translations are primitive and constitute an invariant subgroup of G; the primitive translations are pure translations of the form:

$$(E|t_n) = (E|n_1t_1 + n_2t_2 + n_3t_3) \qquad \text{II.1.5}$$

Here n_1, n_2 and n_3 are integers and t_1, t_2 and t_3 are three linearly independent translations, called basic primitive translations.

From the fact that the primitive translations of a space group G from an invariant subgroup of G, it follows that if $(R \mid t)$ is an element of G then, whenever $(E \mid t_n)$ is a primitive translation, $(E \mid Rt_n)$ is also a primitive translation of G. In fact:

$$(E \mid Rt_n) = (R \mid t)(E \mid t_n)(R \mid t)^{-1} \qquad \text{II.1.6}$$

Equation II.1.6 imposes some restrictions on both rotations and translations of a space group. The rotational parts R of the elements $(R \mid t)$ of a space group can only be proper rotations through integral multiples of 60° and 90° and improper rotations which are products of the mentioned rotations with the inversion. There are only 32 groups of rotations satisfying these conditions, they are called <u>point groups</u>. The periodic structure generated by the primitive translations in a space group is called <u>Bravais lattice</u>. Eq. II.1.6 means that the lattice in a space group must be invariant under the operations of the associated point group. The consequence is that only 14 lattices can exist, (see Koster, 1957).

A lattice and a point group do not specify completely a space group. In fact a non-primitive translation $\vec{\tau}$ may appear in a space group but only in combination with a rotation other than the identity. We can therefore say that the most general element in a space group has the form:

$$(R\,|\,\tau(R)+t) \qquad \text{II.1.7}$$

where $\vec{\tau}(R)$ is either zero or a non-primitive translation and $\vec{t}$ is a primitive translation. Since only primitive translations are associated with the identity rotation, $\vec{\tau}(E) = 0$.

Depending on whether the vector $\tau(R)$ is zero for every R, or is not zero for some R a space group is called symmorphic or non-symmorphic. A symmorphic space group contains the entire point group as a subgroup. A non-symmorphic space group does not contain the entire point group as a subgroup. However, for any space group G the factor group G/T is isomorphic to the point group P of all the rotational parts of the operators of G.

$$\frac{G}{T} = P \qquad \text{II.1.8}$$

Such point group P is said to belong to G. Examples of symmorphic space groups are O_h^1 (simple cubic), O_h^9 (body-centered cubic), T_d^2 (zincblende structure). Examples of non-symmorphic space groups are O_h^7 (diamond structure), D_{6h}^4 (hexagonal close-packed).

From the definition of space group of a crystal as a group of transformations under which the crystal is invariant and whose pure translations form an invariant subgroup it follows that one can define a smallest volume, called unit cell, from which the entire crystal can be reproduced by translation through the primitive translations. A unit cell can be defined in several ways. The simplest way is to take as a unit cell the parallelopiped with edges t_1, t_2 and t_3. But such a unit cell has the disadvantage that it does not necessarily go into itself under the operations of the point group which leaves the lattice invariant. A unit cell which has the symmetry of the point group P is called symmetric unit cell and can be defined in the following way: it is the volume enclosed and bounded by the planes which form the perpendicular bisectors of all lines that extend from a given lattice point to all the remaining lattice points in the crystal.

A concept which plays an important role in the theory of irreducible representations of a space group is that of reciprocal lattice.

If t_1, t_2 and t_3 are the three basic primitive translations of a lattice T, then the basic primitive translations b_1, b_2 and b_3 of its reciprocal lattice are defined by the relations:

$$\vec{t}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \qquad (i,j = 1,2,3) \qquad \text{II.1.9}$$

An important property of the reciprocal lattice corresponding to a given direct lattice is that it is invariant under the same point group operations under which the direct lattice is invariant. This means that if t_i and k_j are primitive translations in the direct and reciprocal lattice respectively, and R is a rotation belonging to the point group which leaves the direct lattice invariant, Rt_i and Rk_j are again primitive translations of the direct and reciprocal lattice respectively. It follows:

$$R\vec{t}_i \cdot \vec{k}_j = 2\pi \times (\text{integer})$$

II.1.10

$$\vec{t}_i \cdot R\vec{k}_j = 2\pi \times (\text{integer})$$

II.2 As we said in the introduction, we intend to study the irreducible representations of the space group D_{4h}^{19} (white tin), therefore we will devote the rest of this chapter to an analysis of its structure.

The space lattice of white tin (Fig. I) is body-centered tetragonal with a basis of two atoms at (0,0,0), $(\frac{t}{\sqrt{2}} \ \frac{t}{\sqrt{2}} \ \frac{s}{2})$ associated with each lattice point, as shown in Fig. II.

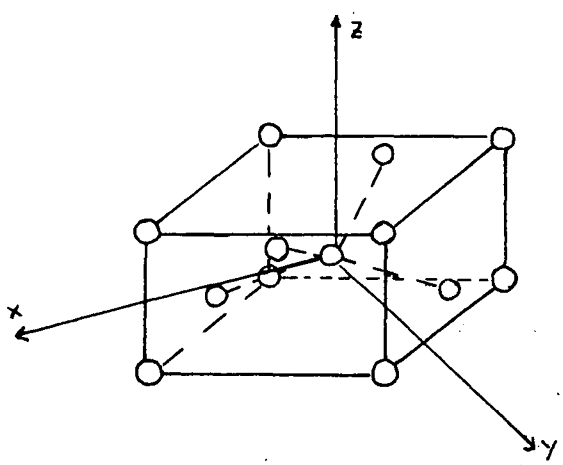

Fig. I Crystal Structure of White Tin

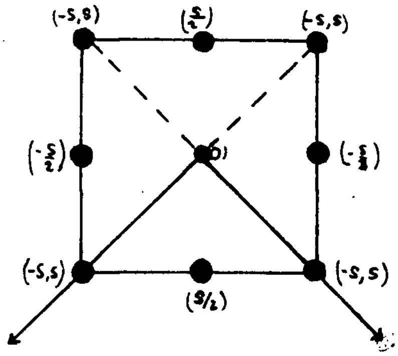

Fig. II Atomic positions in the unit cell of the white tin structure projected on the plane z=0 through the atom in the center of the cell. The symbols in parentheses denote the height of the atoms with respect to the plane z=0. For example, (-s,s) at the upper left corner indicates that along the edge of the cell perpendicular to the plane z=0, there is an atom at z=s and another at z=-s.

Each atom has four nearest neighbours and twelve next nearest neighbours. The lattice constants are:

$$2s = 3.17\ \text{Å} \qquad 2t = 5.82\ \text{Å}\ .$$

The white tin space group is D_{4h}^{19}. Its point group is D_4^h. D_{4h}^{19} is not a symmorphic space group. In fact it contains non-primitive translations in association with some of the elements of D_4^h. All elements of D_4^h which are also elements of the subgroup D_{2d} have no non-primitive translations associated with them. However, the remaining elements of the point group D_4^h occur in combination with a non-primitive translation.

The following operations belong to D_{2d}:

E	identity
S_{4z}, S_{4z}^{-1}	rotation through $\pm\ \pi/2$ about the z-axis followed by a reflection through the plane z=0.
C_{2z}	rotation through π about the z-axis
C_{2x}, C_{2y}	rotations through π about the x- and y-axis
σ_{dxy}, $\sigma_{d\bar{x}y}$	reflections through the planes x=y and x=-y.

The above operations appear in the space group in the form $(R\ |\ t_n)$ where R is a rotation belonging to D_{2d} and t_n is a primitive translation of the body-centered tetragonal lattice.

The remaining operations of D_4^h are:

I	inversion
C_{4z}, C_{4z}^{-1}	rotation through $\pm\ \pi/2$ about the z-axis
C_{2xy}, $C_{2\bar{x}y}$	rotations through π about the two lines x=y z=0 , x=-y z=0
σ_h	reflection through the plane z=0
σ_{vxz}, σ_{vyz}	reflections through the vertical planes y=0, x=0 .

These operations appear in the space group with the non-primitive translation τ :

$$\vec{\tau} = \frac{t}{\sqrt{2}}\left(\vec{i} + \vec{j}\right) + \frac{s}{2}\vec{k} \qquad \text{II.2.1}$$

We have said that white tin has a body-centered tetragonal lattice. This type of Bravais lattice can be regarded as generated by three of the eight vectors extending from the center to the corners of a rectangular solid with a square basis.

Using the coordinate system indicated in Figs. I and II, the three basic primitive translations can be taken to be:

$$\vec{t}_1 = \sqrt{2}\,t\,\vec{j} + s\,\vec{k}$$

$$\vec{t}_2 = \sqrt{2}\,t\,\vec{j} - s\,\vec{k} \qquad \text{II.2.2}$$

$$\vec{t}_3 = \sqrt{2}\,t\,\vec{i} - s\,\vec{k}$$

Since $s < \sqrt{2}\,t$, the symmetrical unit cell of white tin is as shown in Fig. III .

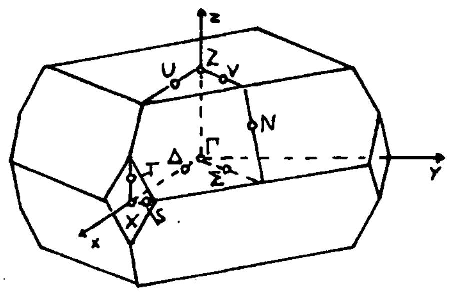

Fig. III Symmetrical Unit Cell for White Tin

To find the reciprocal lattice of the b-c tetragonal lattice we use the relationship II.1.9 where $\vec{t}_1$, $\vec{t}_2$ and $\vec{t}_3$

are given by II.2.2 and b_1, b_2 and b_3 are the unknowns. Solving these three systems of equations one finds:

$$\vec{b}_1 = \frac{\pi}{\sqrt{2}\,t}\left(\vec{i} + \vec{j}\right) + \frac{\pi}{s}\,\vec{k}$$

$$\vec{b}_2 = \frac{\pi}{\sqrt{2}\,t}\left(-\vec{i} + \vec{j}\right) - \frac{\pi}{s}\,\vec{k} \qquad \text{II.2.3}$$

$$b_3 = \frac{\sqrt{2}\,\pi}{t}\,\vec{i}$$

These are the primitive translations in a b-c tetragonal lattice with lattice constants $\sqrt{2}\pi/t$, $\sqrt{2}\pi/t$ and $2\pi/s$. Since $t > s$, then $\sqrt{2}\pi/s > \sqrt{2}\pi/t$. From this last relationship it follows that the symmetrical unit cell in the reciprocal lattice has a different shape from that in the direct lattice. Fig. IV (see Koster, 1957)

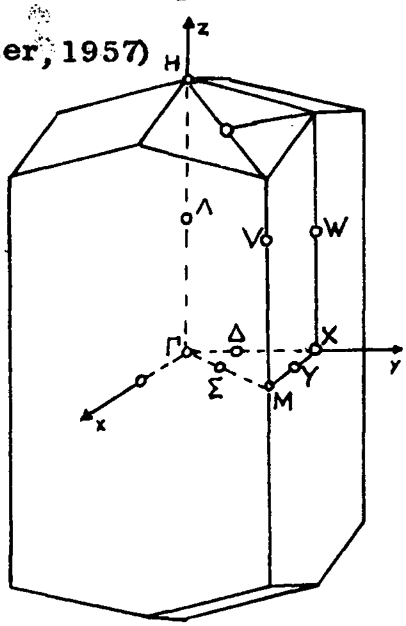

Fig. IV Symmetrical Unit Cell for the Reciprocal Lattice of White Tin

CHAPTER III

Irreducible Representations of Space Groups

Irreducible Representations of the Space Group D_{4h}^{19}

III.1 It is well known (see, for example, Lomont, 1959) that there exists a systematic procedure for finding all the irreducible representations of a group G if all the irreducible representations of an invariant subgroup H of G are given.

This procedure was specialized to the case of space groups by Seitz (1936). However, he restricted himself to general considerations. Bouckaert, Smoluchowski and Wigner (1936) were the first to apply the general theory to specific space groups.

The role of the invariant subgroup H of G when G is a space group, is played by the subgroup of primitive translations T. Therefore in order to apply the general procedure mentioned above, we have first to discuss the irreducible representations of T.

The lattice T is an abelian group, therefore all its irreducible representations are one-dimensional. Its representations (see Lomont) are of the form

$$e^{i\vec{k}\cdot\vec{t}} \qquad \text{III.1.1}$$

where $\vec{k}$ is a real vector and $\vec{t}$ is a translation of T.

From the definition of reciprocal lattice we know that if K_q is a vector of the reciprocal lattice, then $\vec{K}_q\cdot\vec{t}$ = integer $\times\, 2\pi$

and $e^{i\vec{K}_q\cdot\vec{t}} = 1$. It follows that the two representations $e^{i\vec{k}\cdot\vec{t}}$ and $e^{i(\vec{k}+\vec{K}_q)\cdot\vec{t}}$ of a translation $\vec{t}$ are identical.

To obtain one-to-one correspondence between the $\vec{k}$-vectors and the irreducible representations of T, one introduces the concept of the Brillouin zone (B-Z). The B-Z is the symmetrical unit cell in the reciprocal lattice and it has the following properties.

To each point inside the B-Z corresponds a different irreducible representation of the group of pure translations. In fact, two points in the interior of the B-Z cannot differ by a primitive translation of the reciprocal lattice. Not to every point on the surface of the B-Z corresponds a different irreducible representation of the group of pure translations. In fact, every point on the surface is equivalent to at least one other point on the surface. To each point $\vec{k}' = \vec{k} + \vec{K}_q$ outside the B-Z corresponds the same representation of the group of pure translations which corresponds to the point $\vec{k}$ inside the B-Z or on its surface.

After having found in this way all the irreducible representations of the group of pure translations, we can now proceed to applying the systematic procedure for finding the irreducible representations of the space group.

The first step in this procedure is to define for each irreducible representation of the group of pure translations (which means for each k in the B-Z) a group G^k called the "group of the wave vector k". This group G^k is defined as the set of all elements $(R \mid t)$ of G such that $R\vec{k} = \vec{k} + \vec{K}_q$ where $\vec{K}_q$ is a reciprocal lattice vector. This subgroup of G is itself a space group and of course contains T. Hence, T is also an invariant subgroup of G^k.

The second step consists in finding all the irreducible representations of G^k which have the property that the matrices representing pure translations are unit matrices multiplied by a factor of the form $e^{i\vec{k}\cdot\vec{t}}$. Here $\vec{t}$ is any translation in T. Such representations are called "small" or "allowable" representations of G^k.

For points inside the B-Z the only value of K_q for which $R\vec{k} = \vec{k} + \vec{K}_q$ is $\vec{K}_q = 0$. If P^k is the point group belonging to G^k and $\Gamma(R)$ is an irreducible representation of P^k, then an allowable representation of G^k is given (see Koster, 1957) by:

$$\Gamma(R|t) = e^{i\vec{k}\cdot\vec{t}}\,\Gamma(R) \qquad \text{III.1.2}$$

where $(R|t)$ belongs to G^k.

For points on the surface of the B-Z one must distinguish between symmorphic and non-symmorphic space groups.

For a k-vector on the surface of the B-Z of a symmorphic space group Eq. III.1.2 is still valid. But it is not valid for a non-symmorphic space group. In fact, let us consider two elements $(R_j \mid \tau' + t')$ and $(R_i \mid \tau'' + t'')$ of a group G^k when G is a non-symmorphic space group. Here $\vec{\tau}'$ and $\vec{\tau}''$ are non-primitive translations and $\vec{t}'$ and $\vec{t}''$ are elements of T.

Their product is $(R_jR_i|R_j\tau'' + R_jt'' + \tau' + t')$.

Multfplying the matrices representing the two elements and using III.1.2 we obtain:

$$\Gamma(R_j|\tau'+t')\,\Gamma(R_i|\tau''+t'') = e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}')}\Gamma(R_j)e^{i\vec{k}\cdot(\vec{\tau}''+\vec{t}'')}\Gamma(R_i)$$

$$= e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}'+\vec{\tau}''+\vec{t}'')}\,\Gamma(R_jR_i) \qquad \text{III.1.3}$$

The matrix representing the product is:

$$\Gamma(R_jR_i|R_j\tau''+R_jt''+\tau'+t') = e^{i\vec{k}\cdot(R_j\vec{\tau}''+R_j\vec{t}'')}\,e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}')}\Gamma(R_jR_i)$$

$$= e^{iR_j^{-1}\vec{k}\cdot(\vec{\tau}''+\vec{t}'+\vec{\tau}'+\vec{t}'')}\Gamma(R_jR_i)$$

$$= e^{i(\vec{k}+\vec{K}_j)\cdot(\vec{\tau}''+\vec{t}'')}\,e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}')}\Gamma(R_jR_i) \qquad \text{III.1.4}$$

$$= e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}'+\vec{\tau}''+\vec{t}'')}\,\Gamma(R_jR_i)\,e^{i\vec{K}_j\cdot(\vec{\tau}''+\vec{t}'')}$$

$$= e^{i\vec{k}\cdot(\vec{\tau}'+\vec{t}'+\vec{\tau}''+\vec{t}'')}\,\Gamma(R_jR_i)\,e^{i\vec{K}_j\cdot\vec{\tau}''}$$

Because for a non-symmorphic space group $e^{i\vec{K}_j \cdot \vec{\tau}''}$ is not, in general, equal to unity, it follows that when a vector k is on the surface of the B-Z, Eq. III.1.2 does not give the allowable representations of G^k. Therefore a special procedure must be used. But before we go into details about this special procedure, we describe the final step for finding the irreducible representations of the space group G from the allowable representations of G^k.

There is a well known theorem according to which it is possible to construct a representation of a group G from a given representation of the subgroup H of G.

The way of constructing a representation of G from a given representation of H is as follows.

Let g and h be the order of G and H respectively. And let us consider the left cosets of H. If A_1, A_2 ... A_g and B_1, B_2 ... B_h are the elements of G and H respectively, such cosets will be: A_1H, A_2H, ... A_nH with $n = g/h$. The product of these n cosets with an arbitrary but fixed element A of G will be again a set of n cosets which is a permutation of the original set. If then one associates with each element A of G the corresponding permutation matrix, one obtains a representation of the group G by permutation matrices. Such matrices have the property that in each row and each column there is only one element different from zero and this element is equal to unity.

Now, let us consider an arbitrary but fixed element A of G and an element A_i of G which characterizes a coset of H. Their product will be an element of G belonging to a coset, say the l-th coset of $H: AA_i = A_l B_k$. Here B_k is a fixed element of H once A, A_i and A_l have been fixed. Then we associate with the element A a matrix whose i-th, l-th element is the element B_k of the subgroup H. From what we said previously it follows that in each row and each column of the matrix representing the element A there is only one element different from zero. Finally we replace in the matrix so obtained the elements B_k of H by the matrices corresponding to these elements in the given representation of H. In this way one gets a representation of G from a given representation of H.

If G is a space group and H is one of its subgroups G^k, one obtains by this method from a given allowable representation of a subgroup G^k a representation of G. Such representation of G can be proved to be irreducible. Moreover, all the irreducible representations of G will be obtained in this way (for details, see Lomont).

A method for finding the allowable representations of a group G^k of a non-symmorphic space group when the vector k is on the surface of the B-Z has been given by Herring(1942)(The same method is applicable to vectors k ending inside the B-Z.) He studied the non-symmorphic space groups: the space group O_h^7 (diamond structure) and the space group D_{6h}^4 (close-packed hexagonal). We will first explain his method and then we will apply it to the space group D_{4h}^{19} .

If $(E \mid t)$ is an element of G^k such that $\vec{k}\cdot\vec{t} = 2\pi x$(integer), then any element $(R_i \mid t_i)(E \mid t)$ of G^k will be represented, in an allowable representation, by the same matrix as the element $(R_i \mid t_i)$. The set of primitive translations which satisfy the condition $\vec{k}\cdot\vec{t} = 2\pi x$ (integer) constitutes a subgroup of T. This subgroup is called the <u>kernel</u> of the representation of G^k and will be denoted by T^k. Instead of considering the group G^k, Herring considered the factor group G^k/T^k. Since we are looking for those representations of G^k which have the property of being allowable, the elements of G^k/T^k which correspond to the cosets of G^k consisting of only primitive translations must also be represented by unit matrices multiplied by $e^{i\vec{k}\cdot\vec{t}}$.

We now proceed to describing a method of finding the tables of characters of irreducible representations of the various groups G^k/T^k according as the vector k ends in a "point of symmetry", on a "line of symmetry" or in a general point of the boundary of the B-Z. But first of all let us give some definitions.

We will say that a point on the boundary of the B-Z is a "point of symmetry" if the group G^k of the vector k ending in it contains more elements than the group $G^{k'}$ of any neighbouring vector k'.

A "line of symmetry" is a line such that all the vectors k' terminating on it have the same group $G^{k'}$ which contains more elements than the $G^{k''}$ of any k" near the line but not on it.

Points on the surface of the B-Z which are not points of symmetry and which do not belong to a line of symmetry have a group G^k containing a reflection or a glide reflection in addition to the translation group.

Let us now find the tables of characters for the group G^k/T^k of a point of symmetry.

The elements of the factor group are cosets of the form $(R \mid t)T^k$ where $\vec{t}$ can be 0 (a non-primitive translation τ) or a primitive translation not belonging to the kernel (τ plus a primitive translation not belonging to T^k). From now on we will indicate a coset $(R \mid t)T^k$ simply by $(R \mid t)$. These cosets (being elements of G^k/T^k) are divided into classes. As usual, we will say that two cosets $(R \mid t)$ and $(S \mid t')$ belong to the same class if there exists another coset $(U \mid t'')$ of G^k/T^k such that:

$$(U \mid t'')^{-1}(R \mid t)(U \mid t'') = (S \mid t') \qquad \text{III.1.5}$$

To find the characters of the various classes we will use Burnside's theorem (Eq. III.1.10 below) and the condition

$$\sum_i h_i |\chi_i|^2 = g \qquad \text{III.1.6}$$

where h_i is the number of elements in the i-th class, χ_i is its character and g is the order of the group G^k/T^k. But let us first derive Burnside's equations which give the characters of the various classes C_i in a group G of elements A_j. Let a class C_i have h_i elements: $C_i = (A_1^{(i)}, A_2^{(i)}, \ldots A_h^{(i)})$. It is known (see Lomont 1959) that every product C_iC_k of two classes of a group G can be decomposed into a sum of classes, i.e.,

$$C_i C_k = \sum_{l=1}^{r} a_{ikl} C_l \qquad \text{III.1.7}$$

Since the matrix representing the class C_i commutes with all the matrices representing the elements A of G, it follows from Schur's lemma that $M(C_i) = \eta_i I_n$ where η_i is a proportionality factor and I_n is the unit matrix of dimension n. Therefore from III.1.7 we obtain:

$$(\eta_i I_n)(\eta_k I_n) = \sum_{l=1}^{r} a_{ikl} (\eta_l I_n)$$

or

$$\eta_i \eta_k = \sum_{l=1}^{r} a_{ikl} \eta_l \qquad \text{III.1.8}$$

On the other hand in a representation of dimension n, the character of $M(C_i)$ is $\eta_i n$ and since the character of $M(C_i)$ must also be equal to the sum of the characters of the matrices of the elements $A_1^{(i)}, A_2^{(i)}, \ldots A_h^{(i)}$ it follows:

$$\eta_i n = h_i \chi_i$$

or

$$\eta_i = \frac{h_i \chi_i}{n} \qquad \text{III.1.9}$$

Combining III.1.8 and III.1.9 we obtain:

$$\frac{h_i \chi_i}{n} \cdot \frac{h_k \chi_k}{n} = \sum_{l=1}^{r} a_{ikl} \frac{h_l \chi_l}{n} \qquad \text{III.1.10}$$

where n is the character of the identity element. Eqs. III.1.10 are Burnside's equations.

It is not always necessary to consider and solve the complete set of equations III.1.6 and III.1.10 to find the table of characters of a group G^k/T^k. In fact, let $(E \mid t_1)$ be a primitive translation not belonging to T^k; if it happens that for two cosets A' and A" belonging to the same class C_j

$$(E \mid t_1) A' = A'' \qquad \text{III.1.11}$$

then the character of the class C_j is zero.

The proof of this statement is as follows. From III.1.11 one gets:

$$\chi(E \mid t_1) \chi_j = \chi_j \; . \qquad \text{III.1.12}$$

We are looking for those representations of G^k for which the matrices corresponding to pure translations $(E \mid t)$ are of the form $e^{i\vec{k}\cdot\vec{t}} I_n$. In other words $\chi(E \mid t_1) \neq 0$, therefore III.1.12 gives $\chi_j = 0$.

When such cases occur, the number of equations to be solved is evidently reduced.

From the way the tables of characters are constructed one can conclude that all the irreducible representations found are allowable irreducible representations of G^k/T^k.

Now, let us consider a vector k' ending on a symmetry line of the surface of the B-Z. A symmetry line goes always through a point of symmetry. We define the kernel $T^{k'}$ of the group $G^{k'}$ as $\vec{k}'$ approaches the point of symmetry $\vec{k}$. $T^{k'}$ is the set of all primitive translations t' such that $e^{i\vec{k}'\cdot\vec{t}'}$ as $\vec{k}'\to\vec{k}$. Again one can construct the classes of $G^{k'}/T^{k'}$ as $\vec{k}'\to\vec{k}$ and find their characters by means of III.1.6, III.1.10 and III.1.12. The tables so obtained are the limits of the characters of $G^{k'}/T^{k'}$ as $\vec{k}'\to\vec{k}$.

Finally, for a general point on the surface of the B-Z there can be at most two irreducible representations of a group G^k. These are one-dimensional representations and can be constructed by inspection, (Herring 1942).

As we said previously, from the allowable representations of the various groups G^k one can construct all the irreducible representations of the space group G. If q is the dimension of an allowable representation of G^k, g is the order of the point group P belonging to G and r is the order of the point group P^k belonging to G^k, then the dimension of the corresponding representation of G is $(g/r)q$.

Of course it is desirable to have a criterion to check whether all the allowable representations of a group G^k and hence all the irreducible representations of the space group G corresponding to the vector k have been found. Döring and Zehler (1953) stated that the following condition must be satisfied:

For each group G^k the sum of the squares of the dimensions of its allowable representations must be equal to the order of the point group P^k.

III.2 As has been said, the Brillouin zone of a lattice is the symmetrical unit cell of its reciprocal lattice. The B-Z of the body-centered tetragonal lattice, which is the lattice of the space group D_{4h}^{19}, has been given in Fig. IV. There, points and lines of symmetry have been indicated.

As we said previously, the representations of a group G^k with k inside the B-Z are given by III.1.2. But if one wants to write the tables of characters for points inside the B-Z, one can also consider for each vector k the factor group G^k/T^k and, applying the same rules as for points on the surface of the B-Z, find all its allowable representations.

We will give tables of characters for representations of the various groups G^k with the end point of the vector k wandering inside and on the surface of the B-Z.

We will start considering the groups of vectors k with the end point inside the B-Z.

For a "general" vector k inside the B-Z, the group G^k contains only primitive translations and T^k consists of just one element $\vec{t} = 0$. The representation of G^k is a one by one representation. The irreducible representation of D_{4h}^{19}

corresponding to $\vec{k}$ is 16 by 16 because the order of the point group D_4^h belonging to D_{4h}^{19} is 16.

<u>$\Gamma(0,0,0)$.</u> When $\vec{k} = 0$, G^k is the entire space group G and the kernel is the entire group of translations. Therefore $G^\Gamma/T^\Gamma = G/T$. We know that for any space group G the factor group G/T is isomorphic to the point group P belonging to G. In case of the space group D_{4h}^{19} , G/T is isomorphic to the point group D_4^h . Since all irreducible representations of D_4^h are known, all irreducible representations of G/T are also known and they are allowable representations. See Table I.

<u>$\Delta(0,k_y,0)$.</u> This is a general point on the y-axis which is a line of symmetry for the B-Z. The point group P^Δ is C_{2v}. We will give the limit characters as $\Delta \to \Gamma$ and as $\Delta \to X$.

As $\Delta(0,k_y,0) \to \Gamma(0,0,0)$ the kernel T^Δ is the group of all translations and G^Δ/T is isomorphic to the group C_{2v}.

As $\Delta \to X(0,\pi/\sqrt{2}t,0)$ the kernel T^Δ contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with n_1+n_2=even. The limiting character of an operation $(R \mid t)$ will simply be the character of the same operation R in an irreducible representation of the point group C_{2v} times the limit of $e^{i\vec{\Delta}\cdot\vec{t}}$ as $\Delta \to X$. See Table II.

<u>$\Sigma(k_x,k_y,0)$.</u> This is the general point along the line of symmetry $k_x=k_y$, $k_z=0$. The point group P^Σ is C_{2v}.

For $\Sigma \to \Gamma$ and $\Sigma \to M(\pi/\sqrt{2}t,\pi/\sqrt{2}t,0)$ the remarks made for $\Delta \to \Gamma$ and $\Delta \to X$ are also valid here. See Table III.

<u>$\Lambda(0,0,k_z)$.</u> This is a general point of the line of

symmetry x=y=0. The point group P^{Λ} is C_{4v}. As $\Lambda \rightarrow \Gamma$, the kernel T^{Λ} is the whole group of translations and the factor group G^{Λ}/T is isomorphic to C_{4v}. See Table IV.

Let us consider now the points on the boundary of the B-Z.

<u>$X(0,\pi/\sqrt{2}t,0)$</u>. This is the intersection of the y-axis with the face $y=\pi/\sqrt{2}t$ of the B-Z. The group P^X is D_{2h}. The kernel T^X contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with n_1+n_2=even and n_3=any integer.

Since X is one of the most interesting points on the surface of the B-Z, we will explain in detail the process of finding the irreducible representations of the factor group G^X/T^X.

The elements of G^X/T^X are:

$(E\,|\,0)$, $(E\,|\,t_1)$, $(C_{2z}\,|\,0)$, $(C_{2z}\,|\,t_1)$, $(C_{2x}\,|\,0)$, $(C_{2x}\,|\,t_1)$, $(C_{2y}\,|\,0)$, $(C_{2y}\,|\,t_1)$, $(I\,|\,\tau)$, $(I\,|\,\tau+t_1)$, $(\sigma_h\,|\,\tau)$, $(\sigma_h\,|\,\tau+t_1)$, $(\sigma_{vxz}\,|\,\tau)$, $(\sigma_{vxz}\,|\,\tau+t_1)$, $(\sigma_{vyz}\,|\,\tau)$, $(\sigma_{vyz}\,|\,\tau+t_1)$, where the

rotational parts are elements of D_{2h}, $\vec{\tau}$ is given by II.2.1, $\vec{t}_1$ is given by II.2.2 and represents all primitive translations not belonging to T^X.

To find the classes of G^X/T^X one uses Eq. III.1.5. Only elements with the same rotational part can belong to the same class. In fact, let $(S\,|\,t_S)$ and $(R\,|\,t_R)$ be two different elements of G^X/T^X, then using Eq. III.1.5 it follows:

$$(S|t_S)^{-1}(R|t_R)(S|t_S)=(S^{-1}|-S^{-1}t_S)(RS|Rt_S+t_R)$$

$$=(S^{-1}RS|S^{-1}Rt_S+S^{-1}t_R-S^{-1}t_S) \qquad \text{III.2.1}$$

But in G^X/T^X all the rotational parts of the elements commute, therefore:

$$(S|t_S)^{-1}(R|t_R)(S|t_S)=(R|RS^{-1}t_S+S^{-1}t_R-S^{-1}t_S). \qquad \text{III.2.2}$$

The classes of G^X/T^X are found to be:

	16	
C_1	1	$(E\,|\,0)$
C_2	1	$(E\,|\,t_1)$
C_3	2	$(C_{2z}|\;0,t_1)$
C_4	2	$(C_{2x}\,|\;0,t_1)$
C_5	1	$(C_{2y}|\;0)$
C_6	1	$(C_{2y}|\;t_1)$
C_7	2	$(I\,|\tau,\tau+t_1)$
C_8	2	$(\sigma_h|\;\tau,\tau+t_1)$
C_9	2	$(\sigma_{vxz}|\;\tau,\tau+t_1)$
C_{10}	2	$(\sigma_{vyz}\,|\;\tau,\tau+t_1)$.

From III.1.12 it follows that the characters of C_3, C_4, C_7, C_8, C_9, C_{10} are zero. Using III.1.6, III.1.7, and III.1.10 we can find χ_1, χ_2, χ_5, χ_6,

$$|\chi_1^2| + |\chi_2|^2 + |\chi_5|^2 + |\chi_6|^2 = 16 \qquad \text{III.2.3}$$

If n is the dimension of an allowable irreducible representation of G^X/T^X, the character χ_1 of $(E \mid 0)$ is: $\chi_1 = n$, and the character of $(E \mid t_1)$ is $ne^{i\vec{X}\cdot\vec{t}_1} = -n$; i.e., $\chi_2 = -n$. From $C_2C_5 = C_6$ it follows:

$$\frac{(-n)}{n}\,\frac{\chi_5}{n} = \frac{\chi_6}{n} \qquad \text{or} \qquad -\chi_5 = \chi_6$$

On the other hand: $C_5C_6 = C_2$, therefore:

$$\frac{\chi_5}{n}\cdot\frac{\chi_6}{n} = \frac{(-n)}{n} \qquad \text{or} \qquad \chi_5\chi_6 = -n^2 \quad , \quad -\chi_5^2 = -n^2$$

So, we have:

$$\chi_1 = n \quad , \quad \chi_2 = -n \quad , \quad \chi_5 = \pm n \quad , \quad \chi_6 = \mp n$$

From Eq. III.2.3 it follows:

$$n^2 + (-n)^2 + (\pm n)^2 + (\mp n)^2 = 16 \qquad \text{i.e.,}\ n = 2$$

So we have the two solutions: $\chi_1 = \chi_5 = -\chi_2 = -\chi_6 = 2$ and $\chi_1 = \chi_6 = -\chi_2 = -\chi_5 = 2$. For all the characters of G^X/T^X see Table V.

<u>$M(\pi/\sqrt{2}t, \pi/\sqrt{2}t, 0)$</u>. This is the intersection of the line $k_x = k_y$, $k_z = 0$ with the line $k_x = k_y = \pi/\sqrt{2}t$. The group P^M

is D_4^h . The kernel T^M contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with $n_1+n_2+n_3$=even. The rotational parts of the elements in G^M/T^M do not commute, therefore it is possible that cosets with different rotational parts belong to the same class. For example, the presence of C_{4z}, C_{4z}^{-1}, S_{4z}, S_{4z}^{-1} in D_4^h makes $(C_{2x}|\ 0)$, $(C_{2y}|\ 0)$, $(C_{2x}|\ t_1)$, $(C_{2y}|\ t_1)$ belong to the same class. For the table of characters of G^M/T^M see Table VI.

$N(\pi/2\sqrt{2}t,\pi/2\sqrt{2}t,\pi/2s)$. The coordinates of this point are given by the solution of the following system of equations:

$$\frac{\pi}{\sqrt{2}\,t}X+\frac{\pi}{\sqrt{2}\,t}Y+\frac{\pi}{s}z-\frac{\pi^2}{2t^2}-\frac{\pi^2}{2s^2}=0$$

$$X=Y$$

$$X=\frac{s}{\sqrt{2}\,t}z$$

The group P^N is C_{2h}. The kernel T^N contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ where n_1 is even, and n_2 and n_3 can be any integer. See Table VII.

$W(0,\pi/\sqrt{2}t,k_z)$. This is a general point on the line $k_x=0$, $k_y=\pi/\sqrt{2}t$, which is a symmetry line on the boundary of the B-Z. The group P^W is C_{2v}. As $W\rightarrow X(0,\pi/\sqrt{2}t,0)$ the kernel contains all primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with n_1+n_2=even. See Table VIII.

$V(\pi/\sqrt{2}t,\pi/\sqrt{2}t,k_z)$. This is a general point on the line $k_x=k_y=\pi/\sqrt{2}t$, which is a line of symmetry of the B-Z. The point group P^V is C_{4v}. As $V \to M(\pi/\sqrt{2}t,\pi/\sqrt{2}t,0)$ the kernel T^V contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with $n_1+n_2+n_3$=even. See Table IX.

<u>$Y(k_x,\pi/\sqrt{2}t,0)$.</u> This is a general point on the line $k_y=\pi/\sqrt{2}t$, $k_z=0$, which is a symmetry line on the boundary of the B-Z. The group P^Y is C_{2v}.

As $Y \to X(0,\pi/\sqrt{2}t,0)$ the kernel contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with n_1+n_2=even and n_3 any integer.

As $Y \to M(\pi/\sqrt{2}t,\pi/\sqrt{2}t,0)$ the kernel contains all the primitive translations $n_1\vec{t}_1+n_2\vec{t}_2+n_3\vec{t}_3$ with $n_1+n_2+n_3$=even. See Table X.

The reason why we have considered limit representations of groups G^k of vectors k with their end-point on a symmetry line, (as for example the representations of G^Δ as $\Delta \to \Gamma$ and $\Delta \to X$), is that they are necessary for constructing the so-called compatibility relations, which are of importance in physical applications. What the term "compatibility" means, is explained below.

First we give without proof some statements on continuity properties of representations.

On a line of symmetry the representation Γ^k of G^k is a continuous function of k.

If a line of symmetry terminates in a point k_o of higher symmetry, the group G^k is a subgroup of G^{k_o}.

If, among the matrices of a representation Γ^{k_o} of G^{k_o}, one considers only the matrices of those elements of G^{k_o} which occur also in G^k, we get a representation $\Gamma_{(s)}^{k_o}$ of G^k which is called by Lomont a "subduced" representation of G^k. And, of course, as k k₀ the representation Γ^{k_o} subduces a limit representation $\Gamma^{k \to k_o}$ of G^k. This subduced limit representation of G^k is in general decomposable into a direct sum of allowable irreducible limit representations of G^k:

$$\Gamma_{(s)}^{k_o} = \sum_{\ell} c_{\ell}^{k_o} \Gamma^{k \to k_o} \qquad \text{III.2.4}$$

If $c_{\ell}^{k_o}$ is different from zero the representation $\Gamma_{\ell}^{k \to k_o}$ is said to be "compatible" with the representation Γ^{k_o}.

Compatibility tables follow the tables of characters. Since each compatibility table refers to a fixed point of symmetry k_o, no special symbols for limit representations are necessary (that is, we would write Γ^k instead of $\Gamma^{k \to k_o}$).

TABLE I **Characters of allowable representations of the group of Γ.**

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Γ_9	Γ_{10}
$(E\|0)$	1	1	1	1	2	1	1	1	1	2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	1	1	-1	-1	0	1	1	-1	-1	0
$(C_{2z}\|0)$	1	1	1	1	-2	1	1	1	1	-2
$(C_{2x}, C_{2y}\|0)$	1	-1	1	-1	0	1	-1	1	-1	0
$(C_{2xy}, C_{2\bar{x}y}\|\tau)$	1	-1	-1	1	0	1	-1	-1	1	0
$(I\|\tau)$	1	1	1	1	2	-1	-1	-1	-1	-2
$(S_{4z}, S_{4z}^{-1}\|0)$	1	1	-1	-1	0	-1	-1	1	1	0
$(\sigma_h\|\tau)$	1	1	1	1	-2	-1	-1	-1	-1	2
$(\sigma_{vxz}, \sigma_{vyz}\|\tau)$	1	-1	1	-1	0	-1	1	-1	1	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}\|0)$	1	-1	-1	1	0	-1	1	1	-1	0

TABLE II **Characters of allowable representations of the group of Δ.**

	$\Delta_1(\Gamma)$	$\Delta_2(\Gamma)$	$\Delta_3(\Gamma)$	$\Delta_4(\Gamma)$	$\Delta_1(X)$	$\Delta_2(X)$	$\Delta_3(X)$	$\Delta_4(X)$
$(E\|0)$	1	1	1	1	1	1	1	1
$(C_{2y}\|0)$	1	-1	1	-1	1	-1	1	-1
$(\sigma_h\|\tau)$	1	1	-1	-1	i	i	$-i$	$-i$
$(\sigma_{vyz}\|\tau)$	1	-1	-1	1	i	$-i$	$-i$	i
$(R\|t)\times(E\|t_1)$							$-\chi(R\|t)$	

TABLE III Characters of allowable representations of the group of Σ.

	$\Sigma_1(\Gamma)$	$\Sigma_2(\Gamma)$	$\Sigma_3(\Gamma)$	$\Sigma_4(\Gamma)$	$\Sigma_1(M)$	$\Sigma_2(M)$	$\Sigma_3(M)$	$\Sigma_4(M)$
$(E\|0)$	1	1	1	1	1	1	1	1
$(C_{2xy}\|\tau)$	1	-1	1	-1	-1	1	-1	1
$(\sigma_h\|\tau)$	1	1	-1	-1	-1	-1	1	1
$(\sigma_{d\|xy}\|0)$	1	-1	-1	1	1	-1	-1	1
$(R\|t)\times(E\|t_1)$						$-\chi(R\|t)$		

TABLE IV Characters of allowable representations of the group of Λ.

	$\Lambda_1(\Gamma)$	$\Lambda_2(\Gamma)$	$\Lambda_3(\Gamma)$	$\Lambda_4(\Gamma)$	$\Lambda_5(\Gamma)$
$(E\|0)$	1	1	1	1	2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	1	1	-1	-1	0
$(C_{2z}\|0)$	1	1	1	1	-2
$(\sigma_{vxz}, \sigma_{vyz}\|\tau)$	1	-1	1	-1	0
$(\sigma_{d\|xy}, \sigma_{d\|\bar{x}y}\|0)$	1	-1	-1	1	0

TABLE V Characters of allowable representations of the group of X .

	X_1	X_2
$(E\|0)$	2	2
$(E\|t_1)$	-2	-2
$(C_{2z}\|0,t_1)$	0	0
$(C_{2x}\|0,t_1)$	0	0
$(C_{2y}\|0)$	2	-2
$(C_{2y}\|t_1)$	-2	2
$(I\|\tau,\tau+t_1)$	0	0
$(\sigma_h\|\tau,\tau+t_1)$	0	0
$(\sigma_{vxz}\|\tau,\tau+t_1)$	0	0
$(\sigma_{vyz}\|\tau,\tau+t_1)$	0	0

TABLE VI Characters of allowable representations of the group of M .

	M_1	M_2	M_3	M_4
$(E\|0)$	2	2	2	2
$(E\|t_1)$	-2	-2	-2	-2
$(C_{4z}, C_{4z}^{-1}\|\tau, \tau+t_1)$	0	0	0	0
$(C_{2z}\|0)$	2	2	-2	-2
$(C_{2z}\|t_1)$	-2	-2	2	2
$(C_{2x}, C_{2y}\|0, t_1)$	0	0	0	0
$(C_{2xy}\|\tau), (C_{2\bar{x}y}\|\tau+t_1)$	0	0	2	-2
$(C_{2\bar{x}y}\|\tau), (C_{2xy}\|\tau+t_1)$	0	0	-2	2
$(I\|\tau, \tau+t_1)$	0	0	0	0
$(S_{4z}, S_{4z}^{-1}\|0, t_1)$	0	0	0	0
$(\sigma_h\|\tau, \tau+t_1)$	0	0	0	0
$(\sigma_{vxz}, \sigma_{vyz}\|\tau, \tau+t_1)$	0	0	0	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}\|0)$	2	-2	0	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}\|t_1)$	-2	2	0	0

TABLE VII Characters of allowable representations of the group of N .

	N_1	N_2	N_3	N_4
$(E\|0)$	1	1	1	1
$(E\|t_1)$	-1	-1	-1	-1
$(C_{2\bar{x}y}\|\tau)$	1	-1	1	-1
$(C_{2\bar{x}y}\|\tau+t_1)$	-1	1	-1	1
$(I\|\tau)$	1	1	-1	-1
$(I\|\tau+t_1)$	-1	-1	1	1
$(\sigma_{dxy}\|0)$	1	-1	-1	1
$(\sigma_{dxy}\|t_1)$	-1	1	1	-1

TABLE VIII Characters of allowable representations of the group of W .

	$W_1(x)$
$(E\|0)$	2
$(E\|t_1)$	-2
$(C_{2z}\|0, t_1)$	0
$(\sigma_{vxz}\|\tau, \tau+t_1)$	0
$(\sigma_{vyz}\|\tau, \tau+t_1)$	0

TABLE IX Characters of allowable representations of the group of V .

	$V_1(M)$	$V_2(M)$	$V_3(M)$	$V_4(M)$	$V_5(M)$
$(E\|0)$	1	1	1	1	2
$(E\|t_1)$	-1	-1	-1	-1	-2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	i	$-i$	i	$-i$	0
$(C_{4z}, C_{4z}^{-1}\|\tau+t_1)$	$-i$	i	$-i$	i	0
$(C_{2z}\|0)$	1	1	1	1	-2
$(C_{2z}\|t_1)$	-1	-1	-1	-1	2
$(\sigma_{vxz}, \sigma_{vyz}\|\tau)$	i	i	$-i$	$-i$	0
$(\sigma_{vxz}, \sigma_{vyz}\|\tau+t_1)$	$-i$	$-i$	i	i	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}\|0)$	1	-1	-1	1	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}\|t_1)$	-1	1	1	-1	0

TABLE X Characters of allowable representations of the group of Y .

	$Y_1(X) = Y_1(M)$
$(E\|0)$	2
$(E\|t_1)$	-2
$(C_{2x}\|0, t_1)$	0
$(\sigma_h\|\tau, \tau+t_1)$	0
$(\sigma_{vxz}\|\tau, \tau+t_1)$	0

TABLE XI   Compatibility relations between Γ and Δ, Σ , Λ .

Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Γ_9	Γ_{10}
Δ_1	Δ_2	Δ_1	Δ_2	$\Delta_3+\Delta_4$	Δ_3	Δ_4	Δ_3	Δ_4	$\Delta_1+\Delta_2$
Σ_1	Σ_2	Σ_2	Σ_1	$\Sigma_3+\Sigma_4$	Σ_3	Σ_4	Σ_4	Σ_3	$\Sigma_1+\Sigma_2$
Λ_1	Λ_2	Λ_3	Λ_4	Λ_5	Λ_2	Λ_1	Λ_4	Λ_3	Λ_5

TABLE XII   Compatibility relations between X and Δ, W, Y.

X_1	X_2
$\Delta_1+\Delta_3$	$\Delta_2+\Delta_4$
W_1	W_1
Y_1	Y_1

TABLE XIII   Compatibility relations between M and Σ, V, Y.

M_1	M_2	M_3	M_4
$\Sigma_1+\Sigma_4$	$\Sigma_2+\Sigma_3$	$\Sigma_2+\Sigma_4$	$\Sigma_1+\Sigma_3$
V_1+V_4	V_2+V_3	V_5	V_5
Y_1	Y_1	Y_1	Y_1

CHAPTER IV

Double Space Groups; Their Properties and Representations Irreducible Representations of the Double Space Group D_{4h}^{19}†

IV.1 It is well known that under a rotation R of the coordinate system to which a physical system is referred, a wave function ψ of the system behaves differently depending on whether ψ is only a function of the spatial coordinates x, y and z, or is also a function of the spin coordinate s.

The operator O_R corresponding to the rotation R is a point transformation if the wave function ψ depends only upon the cartesian coordinates of the particles in the system. But if ψ depends also upon the spin of the particles in the system, then the operator O_R is split into two factors. Namely:

$$O_R = U_R \times P_R \qquad \text{IV.1.1}$$

Here P_R affects only the position coordinates in the wave function of the given system, U_R affects only the spin coordinate s. In the specific case of a crystal one is interested in wave functions describing electrons in the crystal or, reducing the N-electron problem to the 1-electron problem, in 1-electron wave functions. Therefore the spin coordinate s can only be +1 or -1.

Hence the matrix $u_2(R)$ representing the operator U_R must be a two by two matrix:

$$u_2(R) = \begin{pmatrix} u(R)_{-1,-1} & u(R)_{-1,1} \\ u(R)_{1,-1} & u(R)_{1,1} \end{pmatrix}$$

Actually, as is well known, two matrices $\pm\, u_2(\alpha,\beta,\gamma)$ operating in the spin space correspond to a rotation R with Euler's angles α, β and γ. These matrices are unitary and unimodular (see for example Wigner, 1959). They are:

$$\pm\, u_2(\alpha,\beta,\gamma) = \begin{pmatrix} e^{-\frac{i\alpha}{2}} \cos\frac{\beta}{2}\, e^{-\frac{i\gamma}{2}} & -e^{-\frac{i\alpha}{2}} \sin\frac{\beta}{2}\, e^{\frac{i\gamma}{2}} \\ e^{\frac{i\alpha}{2}} \sin\frac{\beta}{2}\, e^{-\frac{i\gamma}{2}} & e^{\frac{i\alpha}{2}} \cos\frac{\beta}{2}\, e^{\frac{i\gamma}{2}} \end{pmatrix} \qquad \text{IV.1.2}$$

Considering both the spatial coordinates and the spin coordinates we can say that to each rotation R correspond two direct product matrices:

$$\pm\, u_2(R) \times P(R) \qquad \text{IV.1.3}$$

To the inversion I in the product space correspond the two direct product matrices:

$$\pm\, u_2(E) \times P(I) \qquad \text{IV.1.4}$$

therefore, to an improper rotation IR, which we know is the product of a proper rotation R with inversion I, will correspond the two matrices:

$$\pm u_2(R) \times P(IR) \qquad \text{IV.1.5}$$

Since we are not interested in the dependence of the wave functions on spatial coordinates, we can assume the electron being at the origin of the coordinate system. Hence the group U_2 of all unitary unimodular two-dimensional matrices u_2 is a representation, which is irreducible, of the group R_3 of all real three-dimensional rotations. And since to each element of R_3 there correspond two elements in U_2 it is customary to say that U_2 is a double valued representation of R_3.

What has been said for the group R_3 can be repeated for the group $\mathcal{R}$ of all real non-singular inhomogeneous transformations $(R \mid t)$. As we said in Chapter II, Section II.1, the group R_3 of pure rotations is a subgroup of $\mathcal{R}$. If now we let the two matrices $(\pm u_2(R) \mid 0)$ of U_2 correspond to an element R of R_3 and the two matrices $(\pm u_2(R) \mid t)$ correspond to an element $(R \mid t)$ of $\mathcal{R}$, we will say that the set $\mathcal{U}_2$ of matrices $(\pm u_2(R) \mid t)$ and $(\pm u_2(R) \mid 0)$ is a double valued representation of $\mathcal{R}$. The multiplication of two elements $(u_2(R_1) \mid t_1)$ and $(u_2(R_2) \mid t_2)$ of $\mathcal{U}_2$ is defined by:

$$(u_2(R_1) \mid t_1)(u_2(R_2) \mid t_2) = (u_2(R_1) u_2(R_2) \mid R_1 t_2 + t_1) \qquad \text{IV.1.6}$$

Let us consider now a space group G which we know is a discrete subgroup of $\mathcal{R}$. Since $\mathcal{U}_2$ is a double valued representation of $\mathcal{R}$, to each element of G correspond two matrices in $\mathcal{U}_2$. The set of matrices of $\mathcal{U}_2$ corresponding to the elements of G is a subgroup G^{+} of $\mathcal{U}_2$. It is then possible to define a double space group in the following way: the "double" group $G^{\dagger}$ of a space group G is an abstract group whose elements have the same multiplication table as the matrices of $\mathcal{U}_2$ corresponding to the subgroup G of $\mathcal{R}$.

Rules which help to find the structure of a double space group from the known structure of the corresponding space group were obtained by Elliott (1954). They were obtained by generalizing the rules derived by Opechowski (1940) for double point groups. We shall state them again.

It is well known that to a class C_n of conjugate elements in R_3 there correspond two different classes C_n' and C_n'' in U_2. (A class C_n of conjugate elements in R_3 is made up of all rotations through an angle $2\pi/n$ about all the possible axes). Exception to this rule is the class of rotations through an angle π. To such a class in R_3 corresponds only one class in U_2.

That the elements of C_n' and C_n'' do not belong to a same class of U_2 means simply that there is no element ξ of U_2 such that $\gamma_n' \xi = \xi \gamma_n''$ where γ_n' and γ_n'' are elements of C_n' and C_n'' respectively corresponding to γ_n in C_n.

Let us consider now the group $\mathcal{R}$ whose elements have the form $(R \mid t)$. To a class $\mathcal{C}_n$ of conjugate elements in $\mathcal{R}$ there correspond, in general, two different classes $\mathcal{C}_n'$ and $\mathcal{C}_n''$ in U_2. Since in the group $\mathfrak{U}_2$ there is no element ξ which satisfies the relation $\gamma_n' \xi = \xi \gamma_n''$, there is no rotational part ξ of an element of $\mathcal{U}_2$ which would satisfy the same relation. In other words the translations $\vec{t}$ do not affect the determination of classes in $\mathcal{U}_2$.

Again an exception to this rule is the class $\mathcal{C}_2$ of $\mathcal{R}$ whose elements represent a rotation through π followed by a translation.

We said previously that to a class C_2 of R_3 corresponds always only one class $C_2' \equiv C_2''$ in U_2. In other words there exists an element ξ of U_2 such that $\gamma_2' \xi = \xi \gamma_2''$ is satisfied. As Opechowski (1940) has pointed out ξ is a rotation through π.

In the case of the group $\mathcal{R}$ we can say that to a class $\mathcal{C}_2$ of $\mathcal{R}$ corresponds only one class $\mathcal{C}_2' \equiv \mathcal{C}_2''$ in $\mathcal{U}_2$ if there is an element $(\xi_2 | t)$ such that

$$(\gamma_2' | t')(\xi_2 | t) = (\xi_2 | t)(\gamma_2'' | t') \qquad \text{IV.1.6}$$

where $(\gamma_2' | t')$ and $(\gamma_2'' | t')$ are the elements corresponding to $(\gamma_2 | t')$ of $\mathcal{C}_2$ in $\mathcal{C}_2'$ and $\mathcal{C}_2''$ respectively.

From Eq. IV.1.5 it follows that two conditions must be satisfied:

$$\gamma_2' \xi_2 = \xi_2 \gamma_2'' \quad ; \quad (E - \xi_2)\vec{t}' = (E - \gamma_2')\vec{t} \qquad \text{IV.1.7}$$

Both conditions are satisfied in the case of the group $\mathcal{R}$. In fact $\mathcal{R}$ contains all the elements with any real non-singular three-dimensional matrix and any real three-dimensional vector, and therefore it contains also an element satisfying the conditions given by Eq. IV.1.6.

We can therefore conclude that to a class $\mathcal{C}_2$ of $\mathcal{R}$ corresponds always only one class in $\mathcal{U}_2$.

Let us consider now a space group G. From the properties of the group $\mathcal{R}$ it follows:

1) To each class of G whose elements have a rotational part different from a twofold rotation correspond always two classes of $G^{\dagger}$.

2) To a class $\mathcal{C}_2$ of G corresponds only one class $\mathcal{C}_2' \equiv \mathcal{C}_2''$ of $G^{\dagger}$ if there is a transformation $(\xi_2|\ t)$ with ξ_2 either a twofold rotation about an axis perpendicular to at least one of the axes of the rotations in the elements of $\mathcal{C}_2$ or a reflection in a plane containing at least one of the above mentioned axes and with $\vec{t}$ satisfying the relation $(E-\xi_2)\vec{t}' = (E-\gamma_2')\vec{t}$.

As far as irreducible representations of a double space group are concerned, it is possible to state a few rules similar to those existing for double point groups.

3) Each irreducible representation of G is also an irreducible representation of $G^{\dagger}$.

The proof is just the same as that given by Opechowski for double point groups. If, as Opechowski did, we call "specific" irreducible representation of a double space group $G^{\dagger}$

an irreducible representation of $G^{\dagger}$ which is not an irreducible representation of G, we can say exactly as Opechowski did for the double point groups:

4) A necessary and sufficient condition for an irreducible representation of $G^{\dagger}$ being a specific irreducible representation of $G^{\dagger}$ is that the character, different from zero, of any element $(R \mid t)'$ of $G^{\dagger}$ be equal and of opposite sign to the character of the element $(R \mid t)''$. The proof runs exactly the same way as for the double point groups.

From 4) two rules follow:

4a) When to a class of a space group G correspond two classes in the double space group $G^{\dagger}$, in a specific irreducible representation of $G^{\dagger}$ the two classes have characters which are equal in absolute value but of opposite sign.

4b) When to a class $\mathcal{C}_2$ of a space group G corresponds only one class $\mathcal{C}_2'$ in $G^{\dagger}$, in a specific irreducible representation of $G^{\dagger}$ the class $\mathcal{C}_2'$ has character zero.

IV.2 Using the previous rules to define the classes of a double space group and some of their characters, and using

$\sum_i h_i |\chi_i|^2$ = order of the double space group, and

$\frac{h_i \chi_i}{\chi_E} \cdot \frac{h_l \chi_l}{\chi_E} = \sum a_{ilk} \frac{h_k \chi_k}{\chi_E}$ we can get the tables of characters for the double space group $D_{4h}^{19\dagger}$. See Tables XIV to XXIII. In the tables we will denote the two classes of the double group of a vector $\vec{k}$ corresponding to a class $(R|t)$ of the simple group of the vector $\vec{k}$ by $(R|t)$ and $(\bar{R}|t)$. (According to the notation introduced in the text, one would use $(R|t)'$ and $(R|t)''$.)

The wave functions of electrons, when one considers also their spins, are linear combinations of products of spatial functions with spin functions. Since a spin function transforms as $D_{\frac{1}{2}}$, a total function transforms as the direct product of a single group representation with $D_{\frac{1}{2}}$. This direct product can be decomposed in terms of the specific representations of the double group. In $D_{\frac{1}{2}}$ the character of a rotation through an angle $2\pi/n$ is $2 \cos \pi/n$.

We will give a table of the direct products of the single group representations with $D_{\frac{1}{2}}$ for each point. Some compatibility tables are included.

TABLE XIV Characters of the specific representations of the double group of Γ.

	Γ_{11}	Γ_{12}	Γ_{13}	Γ_{14}
$(E\|0)$	2	2	2	2
$(\bar{E}\|0)$	-2	-2	-2	-2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$(\bar{C}_{4z}, \bar{C}_{4z}^{-1}\|\tau)$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$(C_{2z}, \bar{C}_{2z}\|0)$	0	0	0	0
$(C_{2x}, C_{2y}, \bar{C}_{2x}, \bar{C}_{2y}\|0)$	0	0	0	0
$(C_{2xy}, C_{2\bar{x}y}, \bar{C}_{2xy}, \bar{C}_{2\bar{x}y}\|0)$	0	0	0	0
$(I\|\tau)$	2	2	-2	-2
$(\bar{I}\|\tau)$	-2	-2	2	2
$(S_{4z}, S_{4z}^{-1}\|0)$	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$
$(\bar{S}_{4z}, \bar{S}_{4z}^{-1}\|0)$	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$
$(\sigma_h, \bar{\sigma}_h\|\tau)$	0	0	0	0
$(\sigma_{vxz}, \sigma_{vyz}, \bar{\sigma}_{vxz}, \bar{\sigma}_{vyz}\|\tau)$	0	0	0	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}, \bar{\sigma}_{dxy}, \bar{\sigma}_{d\bar{x}y}\|0)$	0	0	0	0

$\Gamma_1 \times D_{1/2} = \Gamma_2 \times D_{1/2} = \Gamma_{11}$ $\quad \Gamma_5 \times D_{1/2} = \Gamma_{11} + \Gamma_{12}$ $\quad \Gamma_8 \times D_{1/2} = \Gamma_9 \times D_{1/2} = \Gamma_{14}$

$\Gamma_3 \times D_{1/2} = \Gamma_4 \times D_{1/2} = \Gamma_{12}$ $\quad \Gamma_6 \times D_{1/2} = \Gamma_7 \times D_{1/2} = \Gamma_{13}$ $\quad \Gamma_{10} \times D_{1/2} = \Gamma_{13} + \Gamma_{14}$

TABLE XV Characters of the specific representations of the double group of Δ.

	$\Delta_5(\Gamma)$	$\Delta_5(X)$
$(E\|0)$	2	2
$(\bar{E}\|0)$	-2	-2
$(C_{2y}, \bar{C}_{2y}\|0)$	0	0
$(\sigma_{\ell}, \bar{\sigma}_{\ell}\|\tau)$	0	0
$(\sigma_{vyz}, \bar{\sigma}_{vyz}\|\tau)$	0	0
$(R\|t)\times(E\|t_1)$		$-\chi(R\|t)$

$$\Delta_1 \times D_{\frac{1}{2}} = \Delta_2 \times D_{\frac{1}{2}} = \Delta_3 \times D_{\frac{1}{2}} = \Delta_4 \times D_{\frac{1}{2}} = \Delta_5$$

TABLE XVI Characters of the specific representations of the double group of Σ.

	$\Sigma_5(\Gamma)$	$\Sigma_5(M)$
$(E\|0)$	2	2
$(\bar{E}\|0)$	-2	-2
$(C_{2xy}, \bar{C}_{2xy}\|\tau)$	0	0
$(\sigma_{\ell}, \bar{\sigma}_{\ell}\|\tau)$	0	0
$(\sigma_{dxy}, \bar{\sigma}_{dxy}\|0)$	0	0
$(R\|t)\times(E\|t_1)$		$-\chi(R\|t)$

$$\Sigma_1 \times D_{\frac{1}{2}} = \Sigma_2 \times D_{\frac{1}{2}} = \Sigma_3 \times D_{\frac{1}{2}} = \Sigma_4 \times D_{\frac{1}{2}} = \Sigma_5$$

TABLE XVII Characters of the specific representations of the double group of Λ.

	$\Lambda_6(\Gamma)$	$\Lambda_7(\Gamma)$
$(E\|0)$	2	2
$(\bar{E}\|0)$	-2	-2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	$\sqrt{2}$	$-\sqrt{2}$
$(\bar{C}_{4z}, \bar{C}_{4z}^{-1}\|\tau)$	$-\sqrt{2}$	$\sqrt{2}$
$(C_{2z}, \bar{C}_{2z}\|0)$	0	0
$(\sigma_{vxz}, \sigma_{vyz}, \bar{\sigma}_{vxz}, \bar{\sigma}_{vyz}\|\tau)$	0	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}, \bar{\sigma}_{dxy}, \bar{\sigma}_{d\bar{x}y}\|0)$	0	0

$$\Lambda_1 \times D_{1/2} = \Lambda_2 \times D_{1/2} = \Lambda_6$$

$$\Lambda_3 \times D_{1/2} = \Lambda_4 \times D_{1/2} = \Lambda_7$$

$$\Lambda_5 \times D_{1/2} = \Lambda_6 + \Lambda_7$$

TABLE XVIII Characters of the specific representations of the double group of X.

	X_3	X_4
$(E\|0)$	2	2
$(\bar{E}\|0)$	-2	-2
$(E\|t_1)$	-2	-2
$(\bar{E}\|t_1)$	2	2
$(C_{2z}, \bar{C}_{2z}\|0, t_1)$	0	0
$(C_{2x}, \bar{C}_{2x}\|0, t_1)$	0	0
$(C_{2y}, \bar{C}_{2y}\|0)$	0	0
$(I\|\tau, \tau+t_1)$	0	0
$(\bar{I}\|\tau, \tau+t_1)$	0	0
$(\sigma_h, \bar{\sigma}_h\|\tau, \tau+t_1)$	0	0
$(\sigma_{vxz}\|\tau)$, $(\bar{\sigma}_{vxz}\|\tau+t_1)$	2	-2
$(\sigma_{vxz}\|\tau+t_1)$, $(\bar{\sigma}_{vxz}\|\tau)$	-2	2
$(\sigma_{vyz}, \bar{\sigma}_{vyz}\|\tau, \tau+t_1)$	0	0

$$X_1 \times D_{1/2} = X_2 \times D_{\frac{1}{2}} = X_3 + X_4$$

TABLE XIX Characters of the specific representations of the double group of M .

	M_5
$(E\|0)$	4
$(\bar{E}\|0)$	-4
$(E\|t_1)$	-4
$(\bar{E}\|t_1)$	4
$(C_{4z}, C_{4z}^{-1}\|\tau, \tau+t_1)$	0
$(\bar{C}_{4z}, \bar{C}_{4z}^{-1}\|\tau, \tau+t_1)$	0
$(C_{2z}, \bar{C}_{2z}\|0)$	0
$(C_{2z}, \bar{C}_{2z}\|t_1)$	0
$(C_{2x}, C_{2y}, \bar{C}_{2x}, \bar{C}_{2y}\|0, t_1)$	0
$(I\|\tau, \tau+t_1)$	0
$(\bar{I}\|\tau, \tau+t_1)$	0
$(S_{4z}, S_{4z}^{-1}\|0, t_1)$	0
$(\bar{S}_{4z}, \bar{S}_{4z}^{-1}\|0, t_1)$	0
$(\sigma_h, \bar{\sigma}_h\|\tau, \tau+t_1)$	0
$(\sigma_{vxz}, \sigma_{vyz}, \bar{\sigma}_{vxz}, \bar{\sigma}_{vyz}\|\tau, \tau+t_1)$	0
$(C_{2xy}, \bar{C}_{2xy}\|\tau), (C_{2\bar{x}y}, \bar{C}_{2\bar{x}y}\|\tau+t_1)$	0
$(C_{2\bar{x}y}, \bar{C}_{2\bar{x}y}\|\tau), (C_{2xy}, \bar{C}_{2xy}\|\tau+t_1)$	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}, \bar{\sigma}_{dxy}, \bar{\sigma}_{d\bar{x}y}\|0)$	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}, \bar{\sigma}_{dxy}, \bar{\sigma}_{d\bar{x}y}\|t_1)$	0

$M_1 \times D_{1/2} = M_2 \times D_{1/2} = M_3 \times D_{1/2} = M_4 \times D_{1/2} = M_5$

TABLE XX Characters of the specific representations of the double group of N .

	N_5	N_6	N_7	N_8
$(E\|0)$	1	1	1	1
$(\bar{E}\|0)$	-1	-1	-1	-1
$(I\|\tau),(\bar{I}\|\tau+t_1)$	1	1	-1	-1
$(C_{2\bar{x}y}\|\tau),(\bar{C}_{2\bar{x}y}\|\tau+t_1)$	1	-1	1	-1
$(\sigma_{dxy}\|0),(\bar{\sigma}_{dxy}\|t_1)$	1	-1	-1	1
$(R\|t)\times(E\|t_1)$		$-\chi(R\|t)$		

$N_1\times D_{\frac{1}{2}}=N_2\times D_{\frac{1}{2}}=N_5+N_6$ $\qquad$ $N_3\times D_{\frac{1}{2}}=N_4\times D_{\frac{1}{2}}=N_7+N_8$

TABLE XXI Characters of the specific representations of the double group of W .

	$W_2(X)$	$W_3(X)$	$W_4(X)$	$W_5(X)$
$(E\|0)$	1	1	1	1
$(\bar{E}\|0)$	-1	-1	-1	-1
$(C_{2z}\|0),(\bar{C}_{2z}\|t_1)$	1	1	-1	-1
$(\sigma_{vxz}\|\tau),(\bar{\sigma}_{vxz}\|\tau+t_1)$	i	$-i$	i	$-i$
$(\sigma_{vyz}\|\tau),(\bar{\sigma}_{vyz}\|\tau+t_1)$	$-i$	i	i	$-i$
$(R\|t)\times(E\|t_1)$		$-\chi(R\|t)$		

$W_1\times D_{\frac{1}{2}}=W_2+W_3+W_4+W_5$

TABLE XXII Characters of the specific representations of the double group of V .

	$V_6(M)$	$V_7(M)$
$(E\|0)$	2	2
$(\bar{E}\|0)$	-2	-2
$(C_{4z}, C_{4z}^{-1}\|\tau)$	$\sqrt{2}\,i$	$-\sqrt{2}\,i$
$(\bar{C}_{4z}, \bar{C}_{4z}^{-1}\|\tau)$	$-\sqrt{2}\,i$	$\sqrt{2}\,i$
$(C_{2z}, \bar{C}_{2z}\|0)$	0	0
$(\sigma_{vxz}, \sigma_{vyz}, \bar{\sigma}_{vxz}, \bar{\sigma}_{vyz}\|\tau)$	0	0
$(\sigma_{dxy}, \sigma_{d\bar{x}y}, \bar{\sigma}_{dxy}, \bar{\sigma}_{d\bar{x}y}\|0)$	0	0
$(R\|t)\times(E\|t_1)$	$-\chi(R\|t)$	

$V_1 \times D_{\frac{1}{2}} = V_3 \times D_{\frac{1}{2}} = V_6$

$V_2 \times D_{\frac{1}{2}} = V_4 \times D_{\frac{1}{2}} = V_7$

$V_5 \times D_{\frac{1}{2}} = V_6 + V_7$

TABLE XXIII Characters of the specific representations of the double group of Y .

	$Y_2(X)=Y_2(M)$	$Y_3(X)=Y_3(M)$	$Y_4(X)=Y_4(M)$	$Y_5(X)=Y_5(M)$
$(E\|0)$	1	1	1	1
$(\bar{E}\|0)$	-1	-1	-1	-1
$(C_{2x}\|0),(\bar{C}_{2x}\|t_1)$	1	1	-1	-1
$(\sigma_z\|\tau),(\bar{\sigma}_z\|\tau+t_1)$	i	$-i$	i	$-i$
$(\sigma_{vxz}\|\tau),(\bar{\sigma}_{vxz}\|\tau+t_1)$	$-i$	i	i	$-i$
$(R\|t)\times(E\|t_1)$		$-\chi(R\|t)$		

$$Y_1 \times D_{\frac{1}{2}} = Y_2 + Y_3 + Y_4 + Y_5$$

TABLE XXIV Compatibility relations between Γ and Δ, Σ, Λ.

Γ_{11}	Γ_{12}	Γ_{13}	Γ_{14}
Δ_5	Δ_5	Δ_5	Δ_5
Σ_5	Σ_5	Σ_5	Σ_5
Λ_6	Λ_7	Λ_6	Λ_7

TABLE XXV Compatibility relations between M and Σ, V, Y.

$M_5 \rightarrow \Sigma_5 + \Sigma_5$; $M_5 \rightarrow V_6 + V_7$; $M_5 \rightarrow Y_2 + Y_3 + Y_4 + Y_5$

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