THE APPLICATION OF SHUBNIKOV GROUPS TO THE DETERMINATION OF ANTIFERROMAGNETIC STRUCTURES

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ABSTRACT

THE APPLICATION OF SHUBNIKOV GROUPS TO THE DETERMINATION OF ANTIFERROMAGNETIC STRUCTURES

by E. Paul Riedel

Following a brief historical account of the development of black-white group theory in one, two and three dimensions, the results of proton-resonance and x-ray studies are combined with the Shubnikov group theory in enumerating the possible arrangements of the magnetic moments in the antiferromagnetic state of azurite $Cu_3(CO_3)_2(OH)_2$. Four antiferromagnetic symmetry groups are found which describe all such possible arrangements of the magnetic moments.

A description of twinning by merohedry and by reticular merohedry in the 14 ordinary and 22 black-white three-dimensional space lattices is presented. All of the possible merohedry and reticular merohedry twin groups for these lattices are then constructed and listed. Included in this list are 142 new merohedry and 40 new reticular merohedry twin groups.

The antiferromagnetic "T wall" twins in NiO are shown to be pseudo-merohedry twins.

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By

E. Paul Riedel

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TABLE OF CONTENTS

SECTION III

TWINNING BY MEROHEDRY AND RETICULAR MEROHEDRY

Tables

Figures

Section I

Black-White Groups

Introduction

The material in Section I is intended to serve generally as an introduction to the existing theory of black-white crystallographic groups in one, two and three dimensions and specifically as a starting point for the material in Sections II and III. As part of the introduction to Section I, a brief historical outline of the development of these groups and some of their applications is presented. Following this, a Bravais lattice method is described for the construction of the three-dimensional black-white space groups. This method is then illustrated by outlining the derivation of the black-white space groups in one and two dimensions. The three-dimensional triclinic and monoclinic space groups are listed. The point groups which correspond to the space groups are also discussed.

Ordinary crystallographic group theory is concerned with describing the symmetry of objects in space. During approximately the last thirty years an important extension of this theory has been developed which consists essentially of describing the symmetry of these objects when a sign + or - is assigned to them. Such an extension of the theory therefore requires the introduction of new crystallographic operations called antioperations which transform an object in the same

way as an ordinary crystallographic operation but change its sign. Groups which contain antioperations are called anti-groups. Change of color of the objects instead of change of sign is usually more convenient to use in diagrams representing the symmetry of these groups. Antioperations are then called colored operations and ordinary operations are called uncolored operations. Groups which contain one or more colored operations but not the colored identity operation are then called black-white groups. Groups which contain the colored identity operation are called gray groups. Groups which do not contain colored operations are the ordinary crystallographic groups.

The first extension of ordinary crystallographic group theory was made in two dimensions in 1928, and 1929 by Alexander and Herrmann in connection with a study of the possible symmetries of liquid crystals.[1,2] If only one side of a plane is considered, the number of possible periodic symmetries of objects in the plane is described by the ordinary 17 two-dimensional crystallographic space groups. Alexander and Herrmann derived all of the two-dimensional space groups when both sides of the plane are considered to be distinct. They found that 63 new groups as well as the original 17 are necessary to describe all such possible symmetries.

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1. E. Alexander, and K. Herrmann, Z. Kristallogr. 69, 285 (1928).

2. E. Alexander, and K. Herrmann, Z. Kristallogr. 70, 328 (1929).

In 1930 Heesch introduced a "fourth coordinate" to three-dimensional crystallographic group theory.[3] This coordinate had no numerical value associated with it; instead it is represented only by a + or - sign. Thus, the groups which he called "the four-dimensional groups of three-dimensional space" describe the space symmetries of objects in three-dimensional space and in addition label the objects + or - . These groups are today called the Shubnikov Groups. Heesch derived all such new triclinic and monoclinic space groups but did not work out explicitly those of the remaining crystal systems. He did, however, derive 90 new point groups which correspond to the new space groups (all the black-white and gray Shubnikov groups) in the same way as the ordinary 32 point groups correspond to the ordinary 230 space groups. The 122 point groups (the 90 derived by Heesch plus the original 32) will be called the Heesch point groups in the present work.*

Shubnikov[4] (1951) rederived the Heesch point groups and also extended the theory to the study of the symmetries of three-dimensional figures using both crystallographic and non-crystallographic operations.

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3. H. Heesch, Z. Kristallogr. 73, 325 (1930).

* They are usually called the Shubnikov point groups in the literature.

4. A. V. Shubnikov, The Symmetry and Antisymmetry of Finite Figures (in Russian), Moscow: Academy of Sciences (1951).

In 1952 Cochran[5] rederived the black-white plane groups and suggested their applicability to the study of the symmetry of real periodic functions used in crystallography.

The complete extension of the black-white group theory to three dimensions was first accomplished by Zamorzaev[6,7] by a mathematical method in 1953. There are 1421 new space groups, 1191 of which are black-white while the remaining 230 are gray. Zamorzaev named these as well as the original 230 space groups the Shubnikov groups.

The new space groups were rederived by a Bravais lattice method and listed by Belov et al.[8] in 1955. A revised list of these groups was published by the latter authors[9] in 1957.

In their discussion of the symmetry of magnetic crystals, Tavger and Zaitsev (1956) derived 58 magnetic point groups.[10]

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5. W. Cochran, Acta Cryst. 5, 630 (1952).

6. A. M. Zamorzaev, "A Generalisation of the Fedorov Groups." Dissertation(in Russian), Leningrad (1953).

7. A. M. Zamorzaev, Soviet Physics Cryst., Vol. 2, No. 1, 10 (1957).

8. N. V. Belov, N. N. Neronova, and T. S. Smirnova, Trudy Inst. Krist. Akad. Nauk S.S.S.R. 11, 33 (1955).

9. N. V. Belov, N. N. Neronova, and T. S. Smirnova, Soviet Physics Cryst., Vol. 2, No. 3, 311 (1957).

10. B. A. Tavger, and V. M. Zaitsev, J. Exptl. Theoret. Phys. U.S.S.R. 30, 564 (1956).

The 58 point groups derived by Tavger and Zaitsev are isomorphic to the 58 black-white Heesch groups.

The first application of Shubnikov groups to the determination of magnetic structures was given by Donnay et al.[11] in 1958. They proposed a systematic method employing neutron diffraction data in conjunction with the Shubnikov groups to determine the magnetic structure of ferromagnetic and antiferromagnetic crystals. They applied the method to the antiferromagnetic crystal chalcopyrite ($CuFeS_2$). A table showing the effects of ordinary symmetry and antisymmetry operations on magnetic moment vectors is also included.

The Heesch groups were first applied in 1958 to the description of certain types of twinning in crystals by Curien and Le Corre.[12]

The possible point symmetry groups of ferromagnetic and antiferromagnetic crystals were discussed by Tavger in 1959. The point groups imply that only certain directions are possible for a macroscopic magnetic moment with respect to the crystal axes. These directions are listed. Tavger also lists the magnetic point groups for which piezomagnetism is possible.[14]

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11. G. Donnay, L. M. Corliss, J. D. H. Donnay, N. Elliott, and J. M. Hastings, Phys. Rev. 112, 1917 (1958).

12. H. Curien, and Y. Le Corre, Bull. Soc. franc. Minér. Crist. 81, 126 (1958).

13. B. A. Tavger, Soviet Physics Cryst., Vol. 3, No. 3, 341 (1959).

14. B. A. Tavger, Soviet Physics Cryst., Vol. 3, No. 3, 344 (1959).

The possible space groups and their corresponding point groups were listed for ferromagnetic and ferroelectric crystals in 1960 by Neronova and Belov.[15]

No attempt has been made above to include all the papers dealing with black-white groups. More extensive references appear in the review papers by Mackay[16] and Le Corre.[17]

The Bravais-Lattice Method

The method employed by Belov et al. in deriving the black-white and gray Shubnikov groups consists of the following general steps:

1. From the 14 original Bravais lattices which describe all the ordinary translational symmetry groups in three dimensions, 22 new black-white lattices are derived by coloring each translational element in turn in a particular Bravais lattice, considering all possible combinations of colored and uncolored translational elements and eliminating those resulting combinations of elements which lead to identities or do not lead to groups.
2. All combinations of colored and uncolored symmetry elements added to each of the 36 lattices are then

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15. N. N. Neronova and N. V. Belov, Soviet Physics Cryst., Vol. 4, No. 6, 769 (1960).

16. A. L. Mackay, Acta Cryst. 10, 543 (1957).

17. Y. Le Corre, Bull. Soc. franc. Minér. Crist. 81, 120 (1958).

considered. When those sets of elements which possess the properties of a group and various identities between groups are recognized, the 1651 Shubnikov groups result. Ten theorems presented in reference 8 and there employed in this process are listed below.

Theorem 1. The reflection in a plane and then a translation in a direction perpendicular to the plane is equivalent to a reflection (of the same character, i.e., mirror or glide) in a "derived" plane which is parallel to the initial one, but located at half the translation from it. The reflection will be uncolored if the first reflection and translation are both uncolored or both colored; and colored if one of the component operations is colored and the other uncolored.

Theorem 2. If a colored translation is parallel to a plane of symmetry, (m,n,c,g) the plane will simultaneously be colored. If this plane coincides with the cell face XOY then in the presence of a color translation* parallel to the x axis $m \equiv a'$, $n \equiv b'$, $a \equiv m'$ and $b \equiv n'$; in the presence of $\vec{t}'$ parallel to y one obtains $m \equiv b'$, $n \equiv a'$, $a \equiv n'$, $b \equiv m'$. If the color translation lies on a diagonal cut $m \equiv n'$, $n \equiv m'$, $a \equiv b'$ and $b \equiv a'$.

If color translations are available along both axes then $m \equiv n \equiv a' \equiv b'$ and $b \equiv a \equiv m' \equiv n'$.

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*The color (indicated by a prime) translation, $\vec{t}'$, magnitude is half that of the uncolored translation in the same direction, i.e., $2|\vec{t}'_x| = |\vec{t}_x|$.

Theorem 3. If the translation is disposed obliquely relative to a symmetry plane, resolve the translation into components perpendicular and parallel to the plane: The first component determines the derived plane shifting it intact parallel to itself just half its length, the second component determines the additional glide component. The derived plane is colored if the plane and translation giving rise to it differ in color and uncolored if both are the same color.

Theorem 4. An axis of n fold order and a perpendicular translation give rise to a parallel derived axis of the same order and character (rotation, screw, inversion, screw translation). The derived axis passes through the apex of a triangle with an apex angle of 360°/n. The position of the apex is given by the basic construction in the rotation plane. The color of the axis is determined as previously by the color of the elements giving rise to it.

Theorem 5. If there is a rotation or screw axis and a colored translation parallel to it, the axis appears simultaneously as a colored rotation or screw axis.

$2 \times t'_{\parallel} = 2\ (2'_1)$
$2_1 \times t'_{\parallel} = 2_1\ (2')$
$3 \times t'_{\parallel} = 3\ (6')$*
$4 \times t'_{\parallel} = 4\ (4'_2)$
$4 \times t'_{\parallel} = 4_1\ (4'_3)$
$4_2 \times t'_{\parallel} = 4_2\ (4')$
$4_3 \times t'_{\parallel} = 4_3\ (4'_1)$

$6 \times t'_{\parallel} = 6\ (6'_3)$
$6_3 \times t'_{\parallel} = 6_3\ (6')$
$6_1 \times t'_{\parallel} = 6_1\ (6'_4)$
$6_5 \times t'_{\parallel} = 6_5\ (6'_2)$
$6_2 \times t'_{\parallel} = 6_2\ (6'_5)$
$6_4 \times t'_{\parallel} = 6_4\ (6'_1)$

* $6'$ is a new symmetry element. It represents a rotation of 120° followed by a colored translation $t'_{\parallel}$. This element is therfore of 6th order. If this operation is repeated three times, the result is $L_6^3 = t + t_{\parallel} + t'_{\parallel}$. If L_6, L_6, and P are a six-fold rotation, six-fold rotation inversion and P a minor plane perpendicular to L_6, then $L_6^3 = L_2$ and $\dot{L}_6^3 = P$.

Theorem 6. If a translation is directed obliquely to an axis resolve the translation into components perpendicular and parallel to the axis. The first transfers the axis to the apex of a triangle with an apex angle of $360^{\circ}/n$. The position of the apex is given by the basic construction in the rotation plane. The second component merges with the resultant axis.

Remarks: 1. The axis of odd order can only be either uncolored or gray. 2. An axis of 3 or 6-fold order combined with a non-parallel color translation can only be gray.

Theorem 7. Two planes (mirror or glide) intersecting in 30°, 45°, 60° or 90° produce a rotation or screw axis of 6, 4, 3 or 2-fold order in the line of intersection or at a distance and parallel to it; the resultant axis is colored if both planes are of the same color and different if they are of different color.

Theorem 8. If two rotation axes of the second order intersect in an angle of 30°, 45°, 60° or 90°, there appear resultant axes of 6, 4, 3 or 2-fold order perpendicular to the plane of the axes producing them and passing through the point of intersection of the axes producing them. The resultant axis is uncolored if both the axes producing it are of the same color and colored if they are of different color. If one or both of the original axes are screw axes, the resultant axis is displaced 1/4 of the translation along each glide direction.

Remarks: Since one can consider the 6-fold axis as the sum of a three and two-fold axis: $6 = 3+2$, we may write for the colored 6-fold axis $6' = 3+2'$. Similarly:

$$6_1' = 3_1 + 2_1' \qquad 6_5' = 3_2 + 2_1'$$
$$6_2' = 3_1 + 2' \qquad 6_4' = 3_2 + 2'$$
$$6_3' = 3 + 2_1'$$

Theorem 9. As a result of the intersection of three mutually perpendicular planes of symmetry or the intersection of an axis and a perpendicular plane of symmetry, there arises a center of symmetry. If there are an even number of intersecting elements containing half-translation components parallel to coordinate axes, the center is not quite symmetrically located along these axes. The center is colored if the number of colored generating elements is not even and uncolored if the number is even. Associated with the intersection of three planes (or an axis and planes) not in a right angle there appears an inversion axis colored or uncolored depending on the number of colored generating elements.

Theorem 10. The combination of a center of symmetry with a translation produces a resultant center halfway between the translation related centers. The resultant center of symmetry is uncolored if the initial center and translation are both of the same color and colored if one is of a different color.

One-dimensional Space Groups

In order to illustrate the general method outlined above, consider the problem in one dimension. There is only one ordinary lattice in one dimension. It possesses just one translational element of symmetry. The diagram of this lattice is shown below where the open circles represent uncolored lattice points and $\vec{t}$ represents the ordinary operation of translational symmetry.

The only black-white lattice which can be found from this lattice by the above procedure is shown below where dark circles represent black lattice points.

Note that the definition of a colored translation implies that for translations in the same direction

$$|\vec{t}| = 2|\vec{t}'|.$$

This is obviously true in two and three dimensions also.

The two translation lattices shown above may be denoted by the symbols ${}_1p$ and ${}_1p_b$, where the subscript 1 denotes one dimension, p primitive lattice type and b a colored translation in the b direction.

Consider now step two of the process outlined above. The only uncolored symmetry operation which exists in one dimension besides the identity and translation is the inversion center i. Graphically this is denoted by a small circle ○, while i' shall be denoted by ⊘ and a gray center (i.e., an uncolored and colored center superimposed) by ⊘ .

Using the 10th theorem and the lattice ${}_1p$, we find five groups which are listed in Table 1.

Table 1. One-dimensional Space Groups based on on Lattice ${}_1p$.

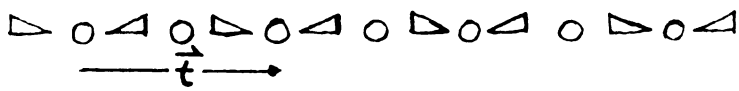
Space Group Symbol	Symmetry Operations or Group Elements
${}_1p1$	$E,\vec{t}$
${}_1p\bar{1}$	$E,\vec{t},i$
${}_1p\bar{1}'$	$E,\vec{t},i'$
${}_1p1'$	$E,E',\vec{t},\vec{t}'$
${}_1p\bar{1}1'$	$E,E',\vec{t},\vec{t}',i,i'$

The groups in Table 1 are shown graphically in Fig. 1 where the triangles are used as objects in general position to show the effect of the group operations.

Fig. 1. Diagrams of the one-dimensional Space Groups based on Lattice $_1p$

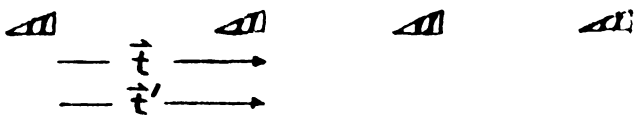
$_1p1$

$_1p\bar{1}$

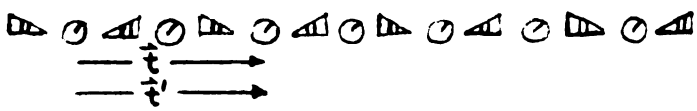


$_1p\bar{1}'$

$_1p1'$

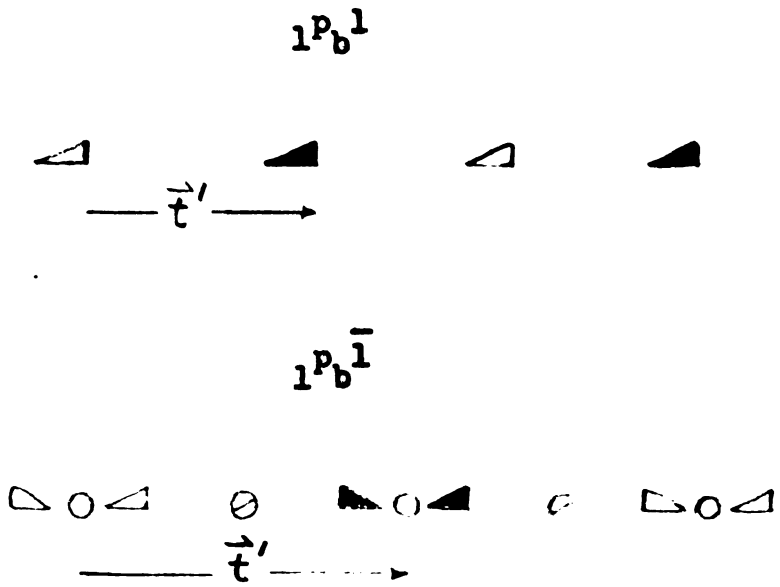


$_1p\bar{1}1'$



Consider next the black-white lattice $_1p_b$. From this two groups are found, $_1p_b1$ with elements E and t' and $_1p_b\bar{1}$ with elements E,t',i and i'. These groups are shown in Fig. 2.

Fig. 2. One-dimensional Space Groups based on Lattice $_1p_b$



In the symbol $_1p_b\bar{1}$ only the uncolored symbol for the inversion, $\bar{1}$, is given; the colored inversion centers being implied by the other elements of symmetry. This method of group notation is used for the Shubnikov groups which have black-white lattices, i.e., only the uncolored elements of symmetry are shown to the right of the lattice symbol. The colored elements in the group are implied by the lattice symbol and the uncolored elements. This method of notation will be used in two dimensions also.

The point group of a crystal describes the directional symmetry of the crystal. The translational part of the symmetry operations contained in the space group do not change directions. Hence, the point group corresponding to any space group may be obtained from the space group by replacing the translational part, if any, of every symmetry operation by the identity operation. The translation $\vec{t}$ is therefore replaced by E, $\vec{t}'$ by E', a glide plane in the c crystallographic direction c by m a mirror plane, c' by m', etc. in obtaining the elements of the point group. The five-point groups obtained in this way from the one-dimensional space groups are listed in Table 2.

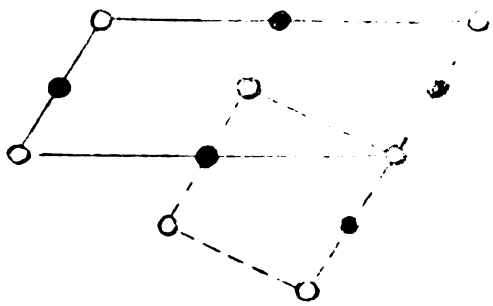
Table 2. Point Groups corresponding to the one-dimensional Space Groups

Space Group Symbol	Corresponding Point Group Symbol	Symmetry Operations or Group Elements
$_1p1$	1	E
$_1p\bar{1}$	$\bar{1}$	E,i
$_1p\bar{1}'$	$\bar{1}'$	E,i'
$_1p1'$	1'	E,E'
$_1p\bar{1}1'$	$\bar{1}1'$	E,i,E',i'
$_1p_b1$	1'	E,E'
$_1p_b\bar{1}$	$\bar{1}1'$	E,E',i,i'

Two-dimensional Space Groups.

There are 17 ordinary, 17 gray and 46 black-white plane groups. In the following description of these groups, we shall continue to follow the methods and, unless otherwise stated, the notation developed by Belov et al.

From the five ordinary lattices in two dimensions five black-white lattices can be derived. These 10 lattices are shown in Fig. 3. Consider, for example, the oblique p lattice. A colored translation along an edge in the a crystallographic direction gives the lattice p_a. The only other possibility is that of a lattice with colored translations along both edges. This gives the lattice shown below (solid lines) which is seen to be identical with p_a (broken lines).



The notation for the ordinary lattices is the same as that given in the "International Tables for X-Ray Crystallography."[18] The black-white lattice notation is the same as that used by Belov et al. except that small instead of capital p's and c's are used in order to denote two dimensions.

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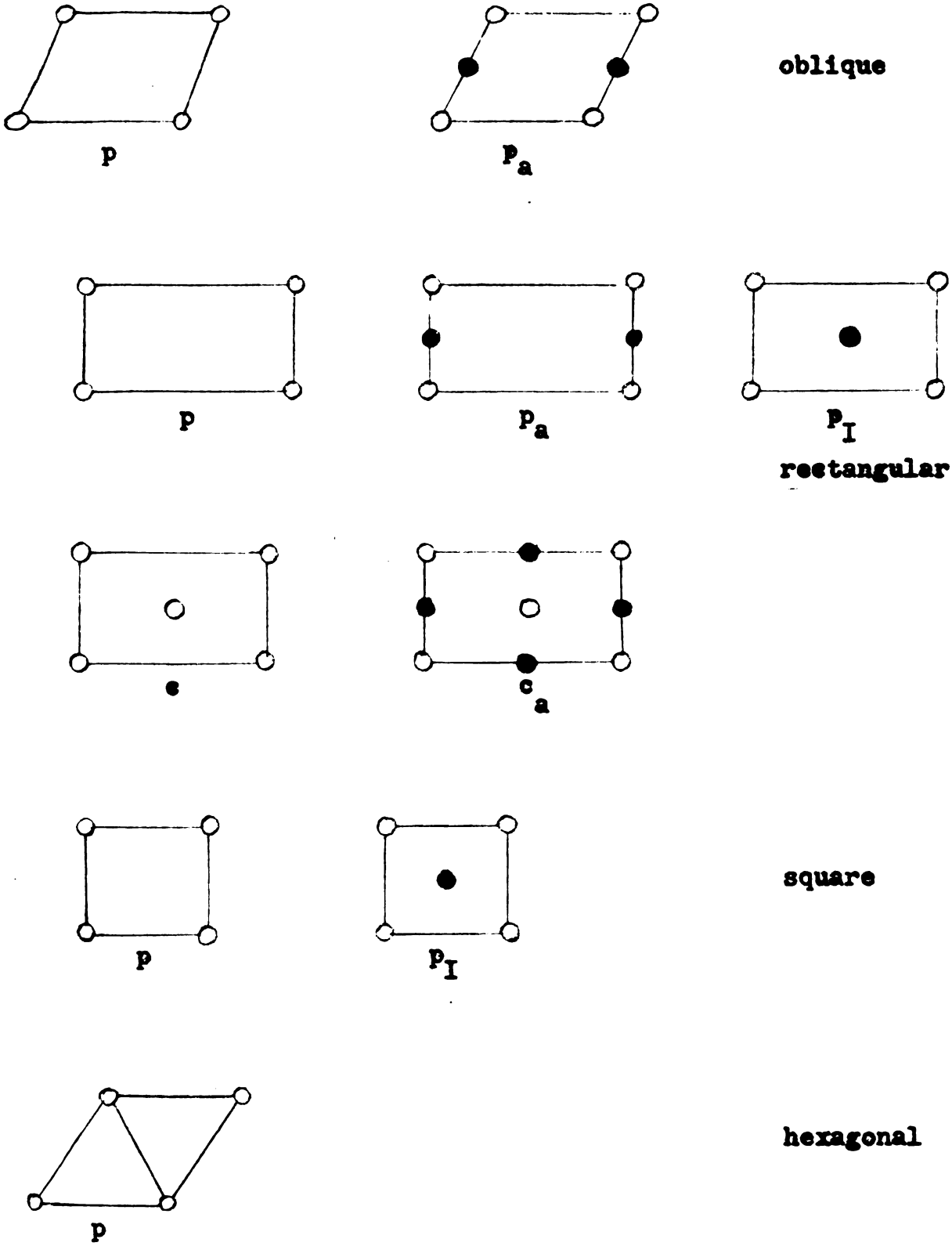
18. International Tables for X-Ray Cryst., Vol. 1, Kynoch Press, Birmingham (1952).

Fig. 3. The five ordinary and five black-white plane Lattices



The lattice symbols have the following meaning:

1. p_a: primitive lattice with a colored translation along the a direction.
2. p_I: primitive lattice with a colored translation along the spacial diagonal of the cell.
3. c_a: centered lattice with colored translations along two non-parallel edges.

This notation is also the same as that used for the Shubnikov groups, except that in this case capital letters such as P and C are used to indicate the lattice types.

The full and short international symbols for the 17 uncolored two-dimensional space groups are shown in Table 3 along with their corresponding point groups. The right-hand column consists of the symbols used in reference 8 for these groups except that in Table 3 the capital P's and C's have been replaced by small letters as mentioned above.

From the original 17 groups 17 gray groups are found by coloring the identity element. Then every element in the group is simultaneously colored and uncolored. These groups are written as p1', p21', pm1', etc.

The 17 original groups also give rise to 26 black-white groups based on ordinary lattices when the elements to the right of the lattice symbol, excluding the identity, are colored in all possible combinations. These groups are shown in Table 4 along with their corresponding point groups.

Table 3. The two-dimensional uncolored Space Groups and their corresponding Point Groups

System and Lattice Symbol	Corresponding Point Group	Space Group Symbols		Belov et al. Space Group Symbol
		Full	Short	
oblique	1	p1	p1	p1
p	2	p211	p2	p2
rectangular	m	p1m1	pm	pm
p		p1g1	pg	pg
and		c1m1	cm	cm
c	2mm	p2mm	pmm	pmm
		p2mg	pmg	pmg
		p2gg	pgg	pgg
		c2mm	cmm	cmm
square	4	p4	p4	p4
p	4mm	p4mm	p4m	p4mm
		p4gm	p4g	p4gm
hexagonal	3	p3	p3	p3
p	3m	p3m1	p3m1	p3m
		p31m	p31m	p31m
	6	p6	p6	p6
	6mm	p6mm	p6m	p6mm

Table 4. The two-dimensional black-white Space Groups based on ordinary Lattices and their corresponding Point Groups

System and Lattice Symbol	Corresponding Point Group	Belov et al. Space Group Symbol
oblique	$2'$	$p2'$
p		
rectangular	m'	pm'
p		pg'
and		cm'
c	$m'm'$	$pm'm'$
		$pg'g'$
		$pm'g'$
		$cm'm'$
	mm'	pmm'
		pgg'
		$pm'g$
		pmg'
		cmm'
hexagonal	$3m'$	$p3m'$
p		$p31m'$
	$6'$	$p6'$
	$6m'm'$	$p6m'm'$
	$6'm'm$	$p6'm'm$
		$p6'mm'$
square	$4'$	$p4'$
p	$4m'm'$	$p4m'm'$
		$p4g'm'$
	$4'mm'$	$p4'mm'$
		$p4'm'm$
		$p4'gm'$
		$p4'g'm$

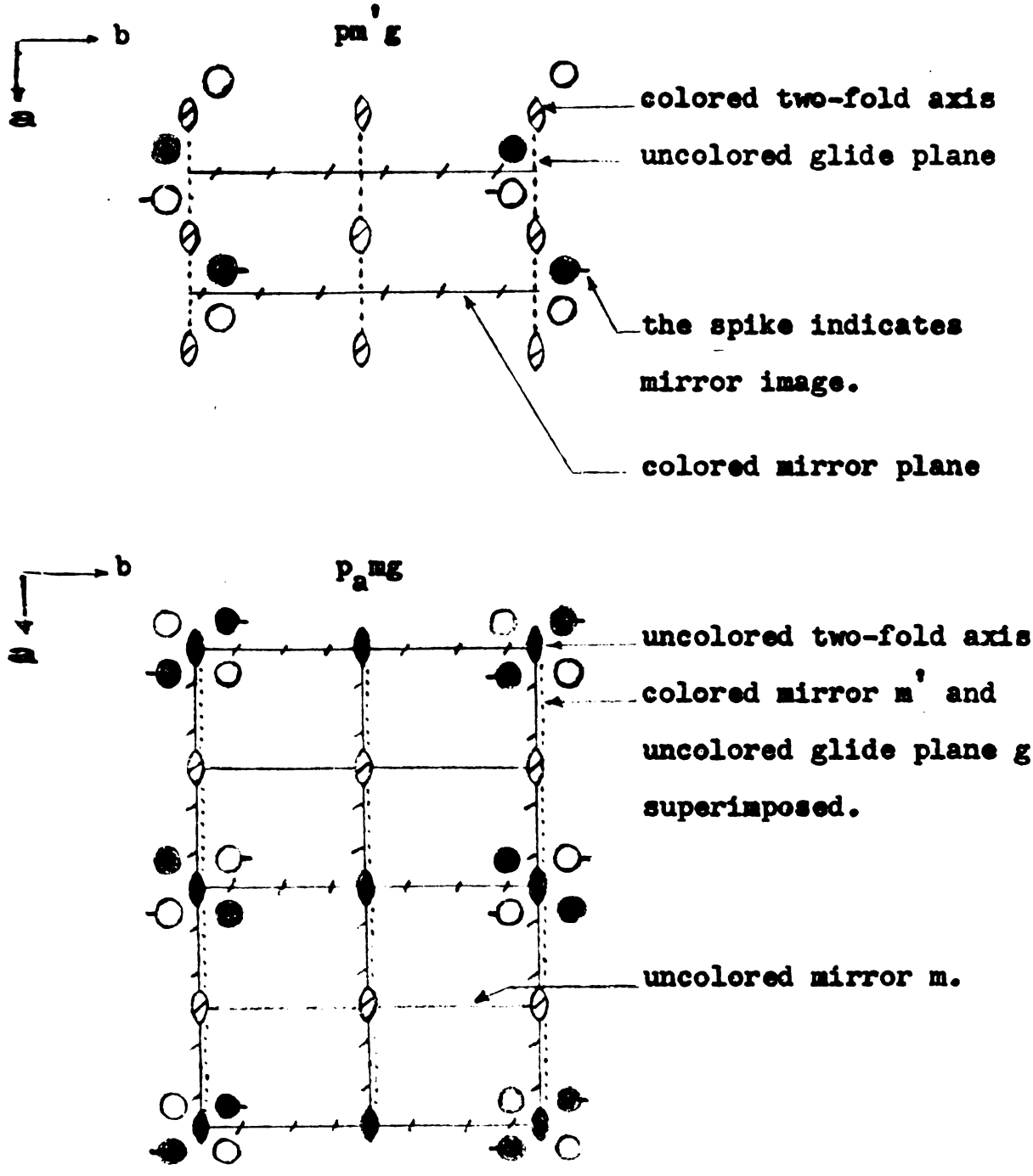
The 20 black-white groups based on black-white lattices are listed in Table 5 along with their corresponding point groups.

Table 5. The two-dimensional Space Groups based on black-white Lattices and their corresponding Point Groups

System and Lattice Symbol	Corresponding Point Group	Belov et al. Space Group Symbol
oblique	$1'$	p_a1
p_a	$21'$	p_a2
rectangular	$m1'$	p_am
p_a		p_a1m
		p_ag
p_I		p_a1g
c_a		p_Im
		p_Ig
		c_am
	$mm1'$	p_amm
		p_agg
		p_amg
		p_agm
		p_Imm
		p_Igg
		p_Img
		c_amm
square	$41'$	p_I4
p_I	$4mm1'$	p_I4mm
		p_I4gm

In order to illustrate the meaning of the symbols for the space groups, the groups $pm'g$ and $p_a mg$ are shown in Fig. 4. There are as yet no standardized symbols for the graphical representation of the antioperations. They will here be represented by cross hatching the uncolored operations as far as is practicable. The uncolored operations will be represented as in "the International Tables for X-Ray Crystallography." For convenience however, all symbols will be defined as they are introduced.

Fig. 4. Diagrams for the Space Groups $pm'g$ and p_amg.

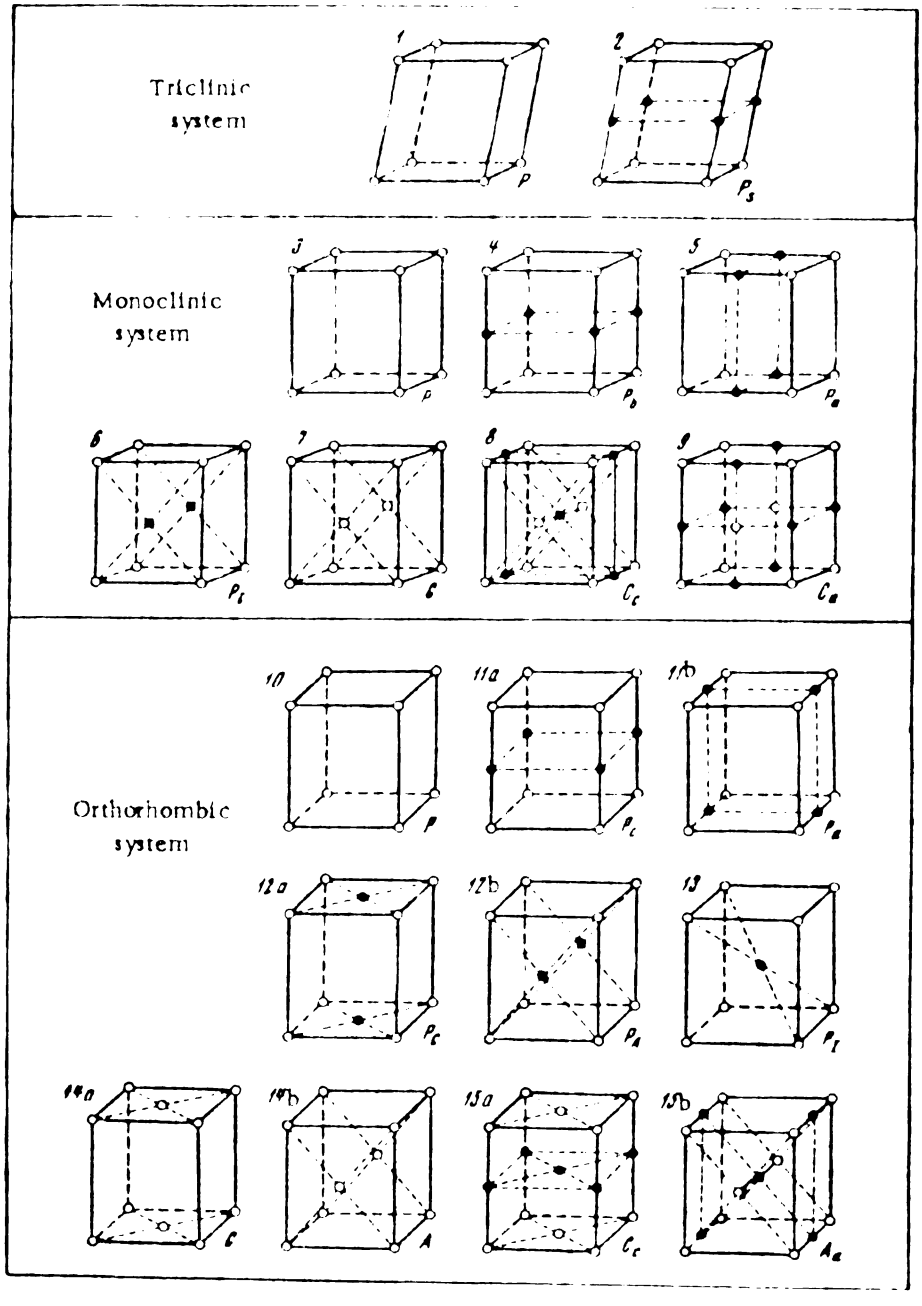


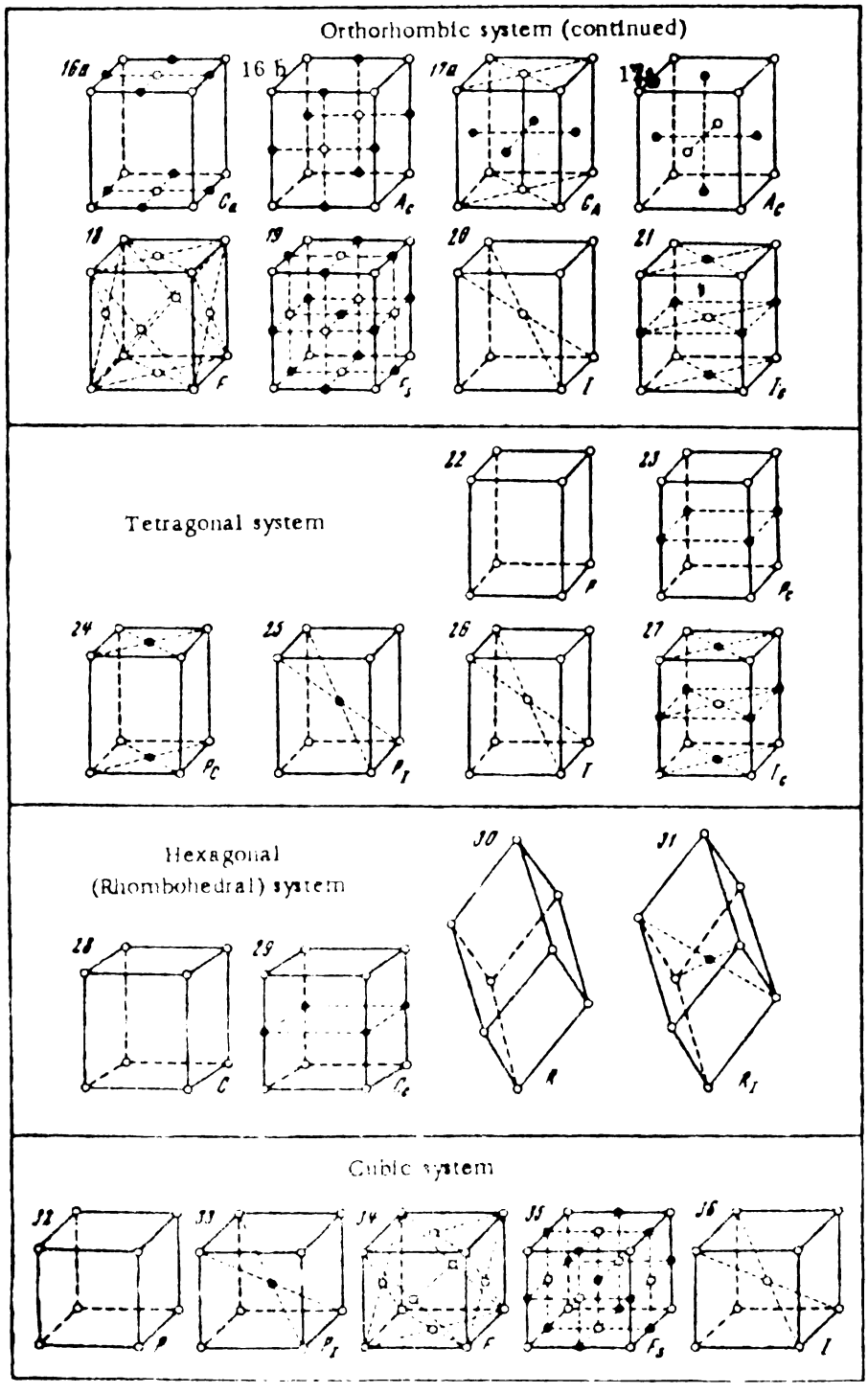
Three-dimensional Space Groups

A reproduction of the 14 original and 22 black-white lattices shown in reference 9 is shown in Fig. 5. The lattice symbols are described below. The numbers to the left refer to the lattice number in Fig. 5.

2.	P_s	colored	translation	along one edge
4.	P_b	"	"	" an edge in the b direction
5.	P_a	"	"	" " " " " a "
6.	P_C	"	"	" the diagonals of the C face
8.	C_c	"	"	in the c direction
9.	C_a	"	"	along edges in the a and b directions
11_a.	P_c	"	"	along an edge in the c direction
12_b.	P_A	"	"	" the diagonals of the A face
13.	P_I	"	"	" " spacial diagonals
15_b.	A_a	"	"	" " a direction
16_b.	A_c	"	"	" edges in the b and c directions
17_b.	A_C	"	"	" the diagonals of the C face
19.	F_s	"	"	" the three edges
21.	I_c	"	"	in the c direction
29.	C_c	"	"	along the c edge
31.	R_I	"	"	" " spacial diagonals

Fig. 5. The 14 original and 22 black-white three-dimensional Lattices




Orthorhombic system (continued)
16a
16 b
17a
17b
18
19
20
21
Tetragonal system
22
23
24
25
26
27
Hexagonal
(Rhombohedral) system
28
29
30
31
Cubic system
32
33
34
35
36

The Shubnikov groups of the triclinic and monoclinic systems are shown in Table 6. Table 6 is a replica of the first part of the complete list in reference 9. Specific examples of a few space groups will be illustrated later in connection with the discussion of azurite.

To the ordinary 230 space groups there correspond 32 point groups. In addition, there are 32 gray and 58 black-white point groups, or 122 Heesch groups in all. All Heesch point groups which contain antioperations have the same general structure. They contain a subgroup of index 2 of unprimed elements, the remaining elements being primed. All 122 Heesch point groups are tabulated in the discussion of the twin problem in the last section. Some examples will also be used in the next section on azurite.

In summary, the number of point and space groups in various categories are listed in Table 7.

Table 6. The Triclinic and Monoclinic Shubnikov Groups

Triclinic System

C_1

1. P1
2. P1'
3. P_s1

C_i

4. $P\bar{1}$
5. $P\bar{1}1'$
6. $P\bar{1}'$
7. $P_s\bar{1}$

Monoclinic System

C_2

1. P2
2. P21'
3. P2'
4. P_a2
5. P_b2
6. P_C2
7. $P2_1$
8. $P2_11'$
9. $P2_1'$
10. P_a2_1
11. P_b2_1
12. P_C2_1
13. C2
14. C21'
15. C2'
16. C_c2
17. C_a2

C_s

18. Pm
19. Pm1'
20. Pm'
21. P_am
22. P_bm
23. P_Cm
24. Pc
25. Pc1'
26. Pc'
27. P_ac
28. P_cc
29. P_bc
30. P_Cc
31. P_Ac
32. Cm
33. Cm1'
34. Cm'
35. C_cm
36. C_am
37. Cc
38. Cc1'
39. Cc'
40. C_cc
41. C_ac

C_{2h}

42. P2/m
43. P2/m1'
44. P2'/m
45. P2/m'
46. P2'/m'
47. P_a2/m
48. P_b2/m
49. P_C2/m
50. $P2_1/m$
51. $P2_1/m1'$
52. $P2_1'/m$
53. $P2_1/m'$
54. $P2_1'/m'$
55. P_a2_1/m
56. P_b2_1/m
57. P_C2_1/m
58. C2/m
59. C2/m1'
60. C2'/m
61. C2/m'
62. C2'/m'
63. C_c2/m
64. C_a2/m
65. P2/c
66. P2/c1'
67. P2'/c
68. P2/c'
69. P2'/c'
70. P_a2/c
71. P_b2/c
72. P_c2/c
73. P_A2/c
74. P_C2/c
75. $P2_1/c$
76. $P2_1/c1'$
77. $P2_1'/c$
78. $P2_1/c'$
79. $P2_1'/c'$
80. P_a2_1/c
81. P_b2_1/c
82. P_c2_1/c
83. P_A2_1/c
84. P_C2_1/c
85. C2/c
86. C2/c1'
87. C2'/c
88. C2/c'
89. C2'/c'
90. C_c2/c
91. C_a2/c

Table 7. The Numbers of ordinary, black-white and gray Space and Point Groups in one, two and three Dimensions

	Number of Dimensions	Number of Point Groups	Number of Space Groups
ordinary	1	2	2
black-white	1	1	3
gray	1	2	2
total		5	7
ordinary	2	10	17
black-white	2	11	46
gray	2	10	17
total		31	80
ordinary	3	32	230
black-white	3	58	1191
gray	3	32	230
total		122	1651

Section II

The Possible Antiferromagnetic Symmetry Groups of Azurite

Introduction

Most of the material in this section has recently been published by the present author and Professor R. D. Spence.[19]

Antiferromagnetic crystals have been shown by neutron diffraction techniques to be periodic structures where the chemical cell which displays only the x-ray symmetry is replaced by the magnetic cell which displays the neutron diffraction symmetry.[20] The magnetic cell represents the symmetry of the magnetic moments, associated with certain ions, as well as the atomic positions.

For any particular magnetic moment direction, there exist two possible senses for the magnetic moment vector. Given a magnetic moment with a certain direction and sense in a unit magnetic cell of an antiferromagnetic crystal, there must also exist in the same cell another magnetic moment with the same magnitude and direction but with opposite sense. Hence, a magnetic moment is subject to both ordinary symmetry and antisymmetry operations where the change of sign operation which characterizes an operation of antisymmetry is here interpreted as an operator R which reverses

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19. E. P. Riedel and R. D. Spence, Physica 26, 1174 (1960).

20. See for example: C. G. Shull and E. O. Wollan, Solid State Physics edited by F. Seitz and D. Turnbull, (Academic Press, New York, 1960), Vol. 2, p. 137.

the sense of a magnetic moment vector. Thus, an antioperation transforms a magnetic moment vector in the same way as an ordinary crystallographic operation followed by a reversal of the sense of the magnetic moment vector.

Two properties of the R operator are implied by the above. R must commute with every symmetry operation and $R^2=E$.

The first published application of Shubnikov groups to the description of an antiferromagnetic crystal appeared in a paper by Donnay et al.[21] Here x-ray and neutron diffraction data were used together with the Shubnikov group theory to find the magnetic structure of chalcopyrite, $CuFeS_2$.

Proton resonance studies of the monoclinic crystal azurite $Cu_3(CO_3)_2(OH)_2$ have shown it to be antiferromagnetic below 1.86°K.[22] In this section, the results of recent proton resonance* and x-ray studies will be combined with the theory of Shubnikov groups in order to enumerate the various possible arrangements of the magnetic moments in the antiferromagnetic state.

The general method used to do this is new. Briefly, it consists of the following. First, the point group symmetry of the local magnetic field vectors at the proton positions

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[21] Donnay et al., op. cit.

[22] R. D. Spence and R. D. Ewing, Physical Rev. 112, 1544 (1958).

* performed by Professor R. D. Spence

is found in the antiferromagnetic state. The magnetic field is an axial vector. The operations of a point group however must transform all axial vectors in exactly the same way. Therefore, the point symmetry of the local field vectors must also be the point symmetry of the magnetic moment vectors (which are also axial vectors) associated with the magnetic ions in the crystal. The Shubnikov space group which represents the symmetry of the magnetic cell must also transform all axial vectors in the same way. It must therefore have as a corresponding Heesch point group one which permits the observed axial vector point symmetry. This space group must also permit the same number of protons which are observed to experience different local magnetic fields. The imposition of these requirements on all Shubnikov groups which do not violate the observed x-ray symmetry of the crystal leads in the case of azurite to four possible antiferromagnetic symmetry groups.

Proton Resonance Data

Figs. 6a, 6b and 6c show the angular dependence of the proton resonance lines in the antiferromagnetic state of azurite in the a'-c, b-c, b-a' (a' perpendicular to c) planes. From the figures, it is clear that in the magnetic unit cell there exist eight protons all with different local magnetic fields. The local fields arising from the copper ions were found by fitting the data to the relation

$$\frac{\nu-\nu_0}{\nu_0} = \left\{1+\left(\frac{H_\ell}{H_0}\right)^2 + 2\frac{H_\ell}{H_0}\cos\Theta\right\}^{1/2} - 1$$

where ν_0 is the frequency of the free proton resonance in

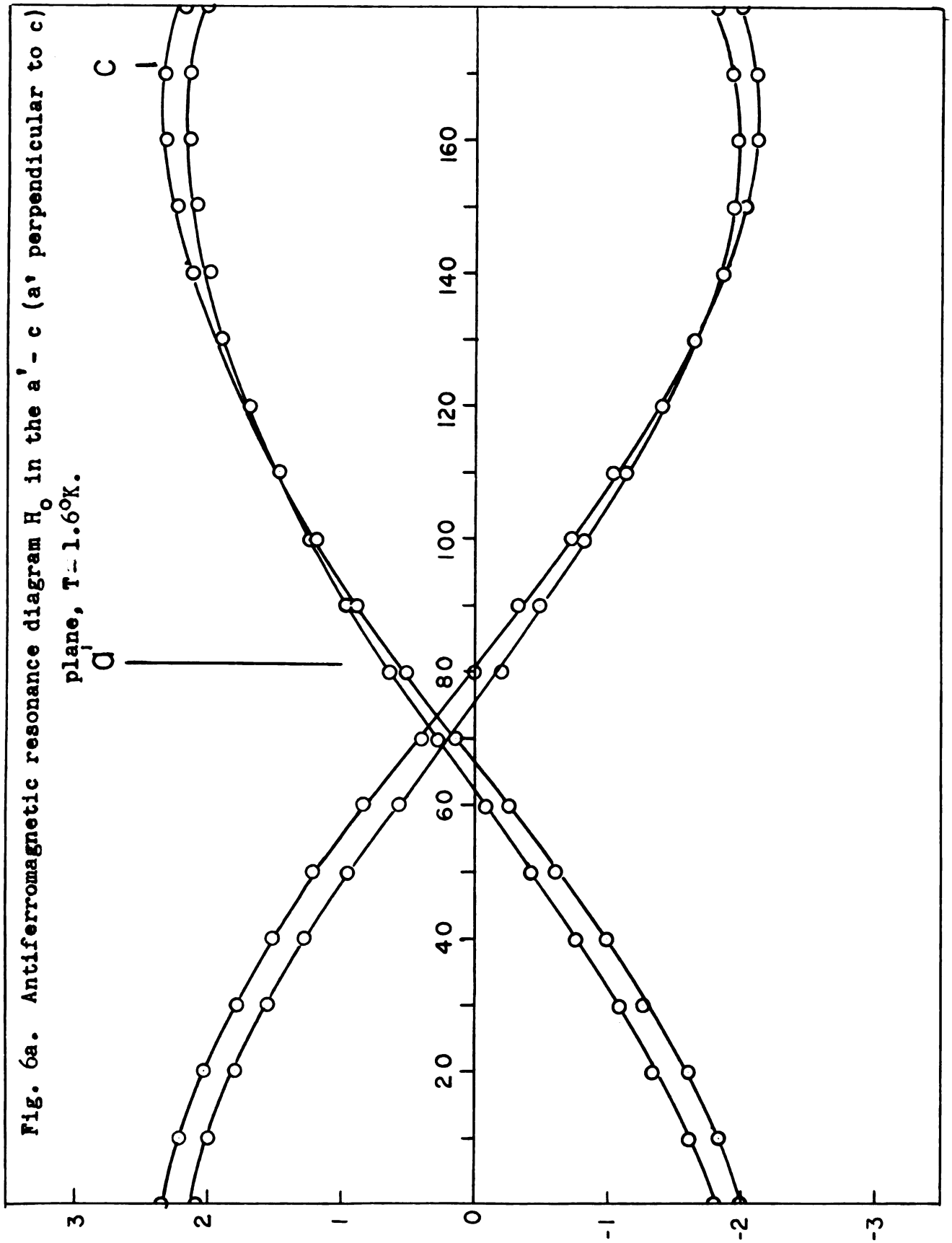


Fig. 6a. Antiferromagnetic resonance diagram H_o in the a' - c (a' perpendicular to c) plane, T- 1.6°K.

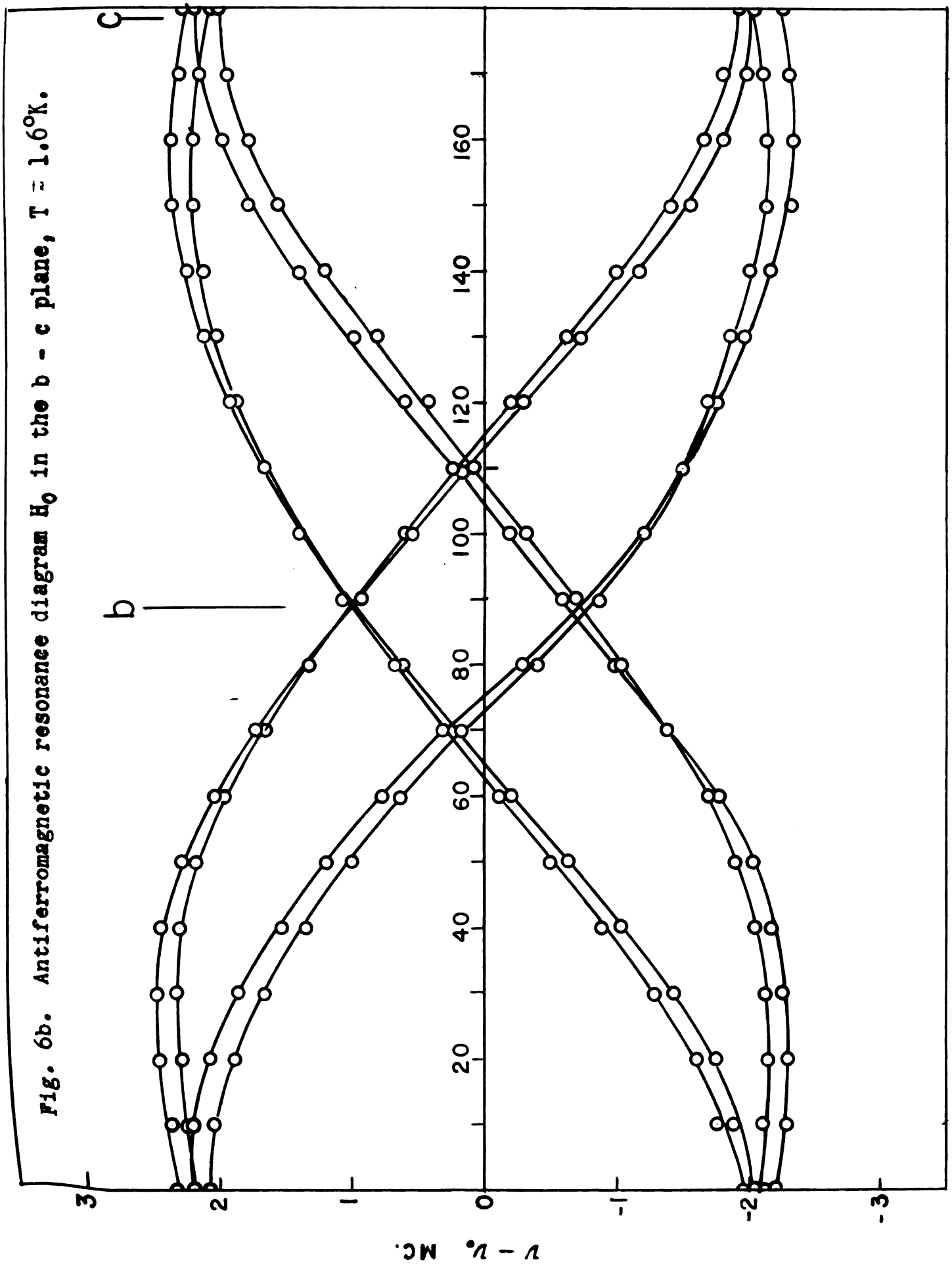


Fig. 6b. Antiferromagnetic resonance diagram H_0 in the b - c plane, T = 1.6°K.

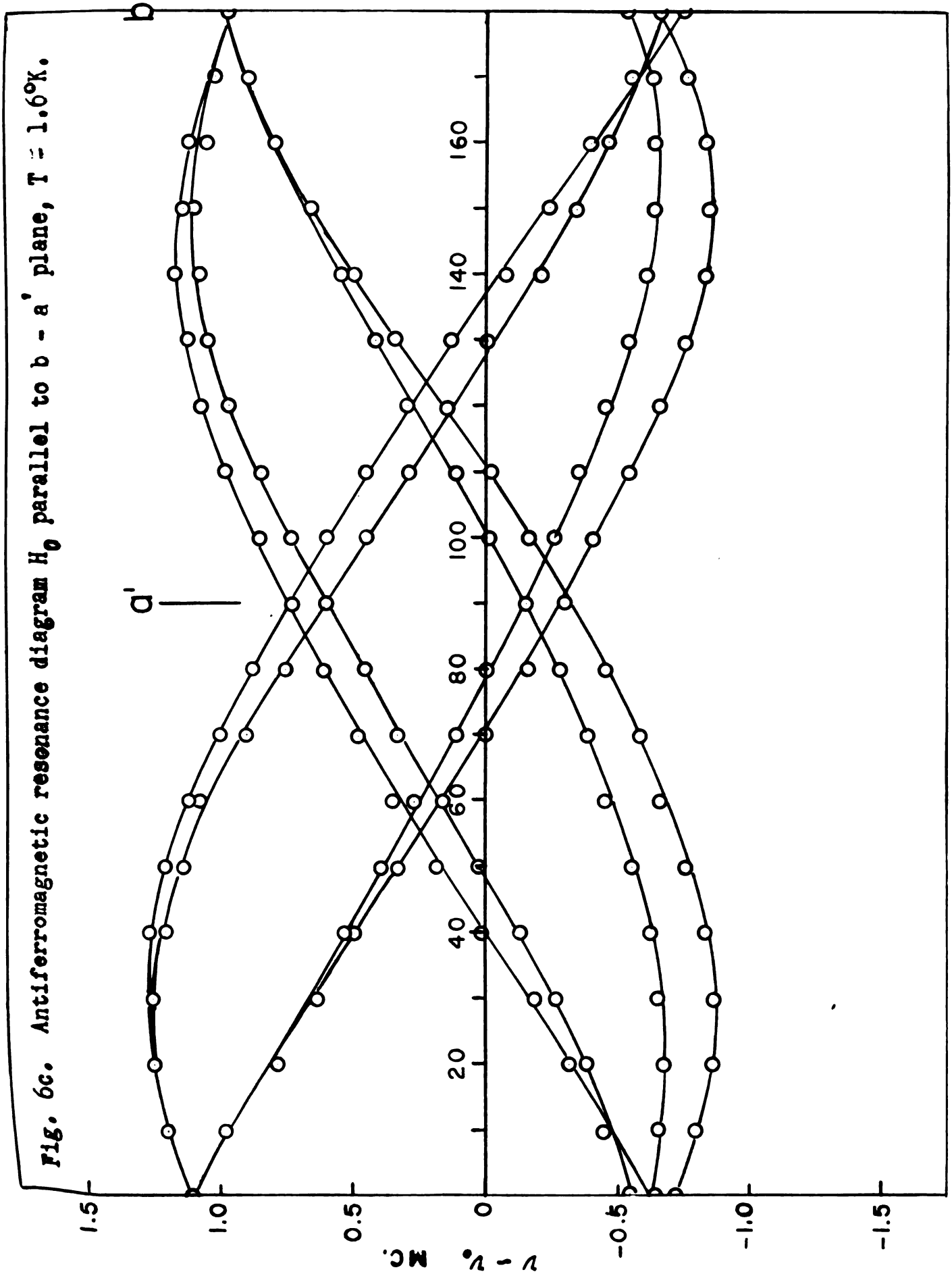


Fig. 6c. Antiferromagnetic resonance diagram H_0 parallel to b - a' plane, T = 1.6°K.

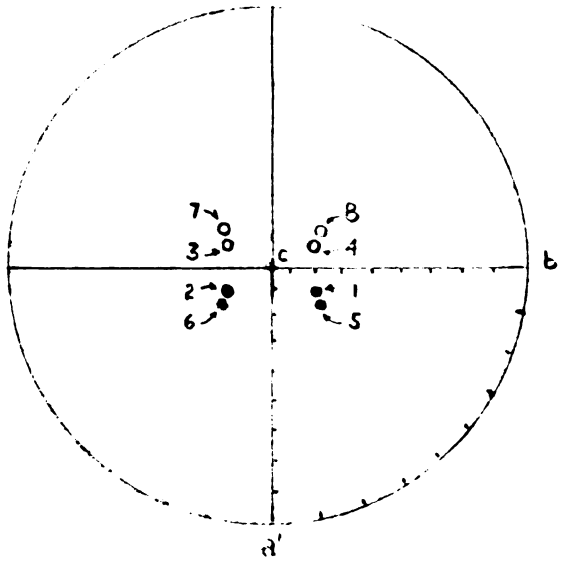
the dc magnetic field H_o and Θ is the angle between H_o and the local field H_ℓ. A derivation of this equation is given in the appendix. The data in Figs. 6a, 6b, and 6c were taken with $H_o = 3430$ gauss and $T = 1.6^\circ K$. The magnitudes and orientations of the local fields are given in Table 8, where $\ominus$ is measured from the c axis and ϕ from the a'-c plane.

Table 8. Local Magnetic Field Vectors at Proton Positions

ℓ	H (gauss)	$\ominus$	ϕ
1	580	23°	62°
2	580	23°	298°
3	580	157°	242°
4	580	157°	118°
5	545	27°	56°
6	545	27°	304°
7	545	153°	236°
8	545	153°	124°

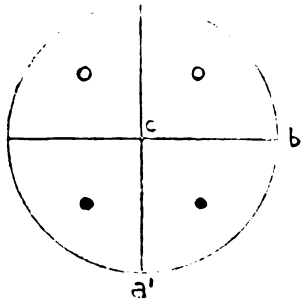
The angular relations between the directions of the local field vectors in the crystal can be conveniently represented by a stereographic projection as shown in Fig. 7. The usual crystallographic convention has been employed in Fig. 7, i.e., vectors in the upper hemisphere are projected through the south pole and indicated by solid circles while vectors in the lower hemisphere are indicated by open circles. In considering the symmetry of Fig. 7, one must bear in mind that it represents angular relations between axial vectors rather than polar vectors which are commonly shown in

Fig. 7. Stereographic Projection of the Local Field Vectors in Table 8.



crystallographic applications of stereographic projections. Since the magnetic moment vectors of the copper ions are axial vectors, they must be transformed by the symmetry operations of the crystal in exactly the same way as are the local field vectors. Hence the point symmetry of any particular magnetic moment vector in the antiferromagnetic state of azurite may be represented as shown in Fig. 8.

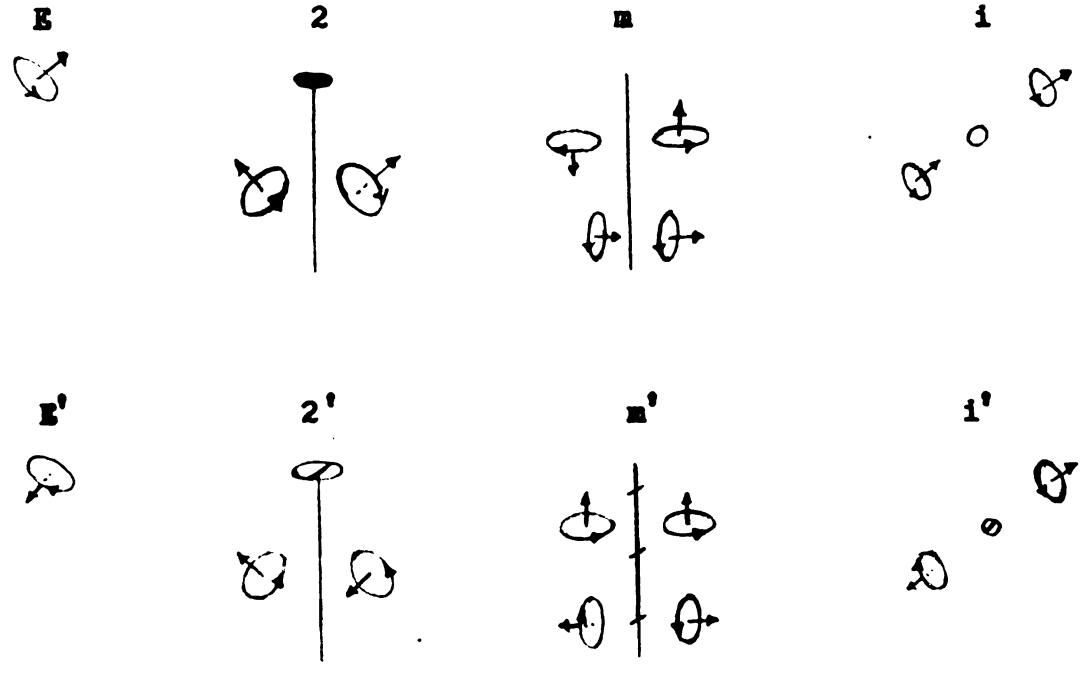
Fig. 8. Point Symmetry of a Magnetic Moment Vector in the Antiferromagnetic State of Azurite.



Point Group Operations

Diagrams showing the effect of some ordinary and anti-symmetry operations on magnetic moment vectors have been constructed by Donnay et al.[23] Some of these are shown in Fig. 9. (A few slight changes in the graphical symbols of some of the operations have been made).

Fig. 9. The Effect of some symmetry Operations on Magnetic Moment Vectors



The effect of the symmetry operations of the Heesch point groups of the triclinic and monoclinic systems on a single arbitrarily oriented axial vector is shown in Figs. 10 and 11 respectively.

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[23] Donnay et al., op. cit. p.1918

Fig. 10. Symmetry of an Axial Vector under the Triclinic Heesch Point Groups

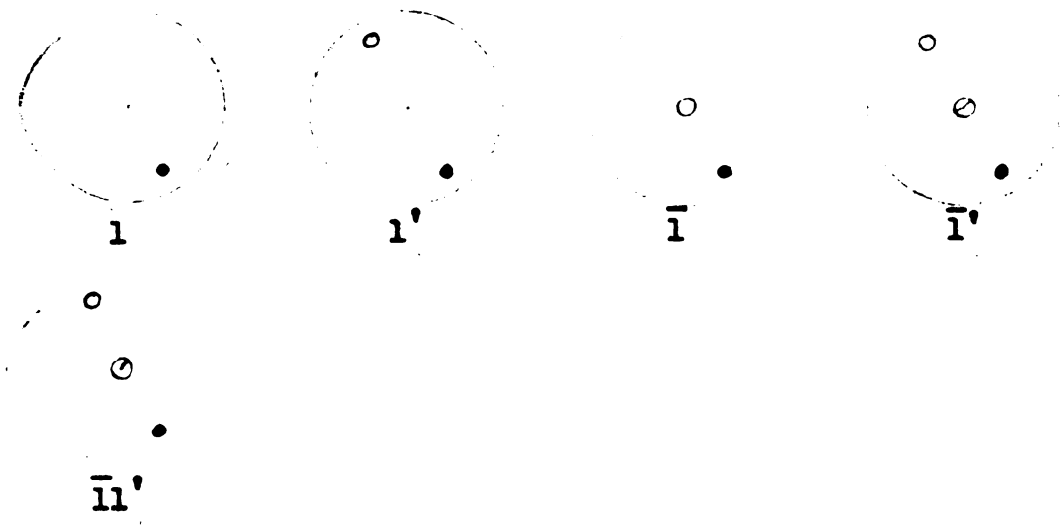
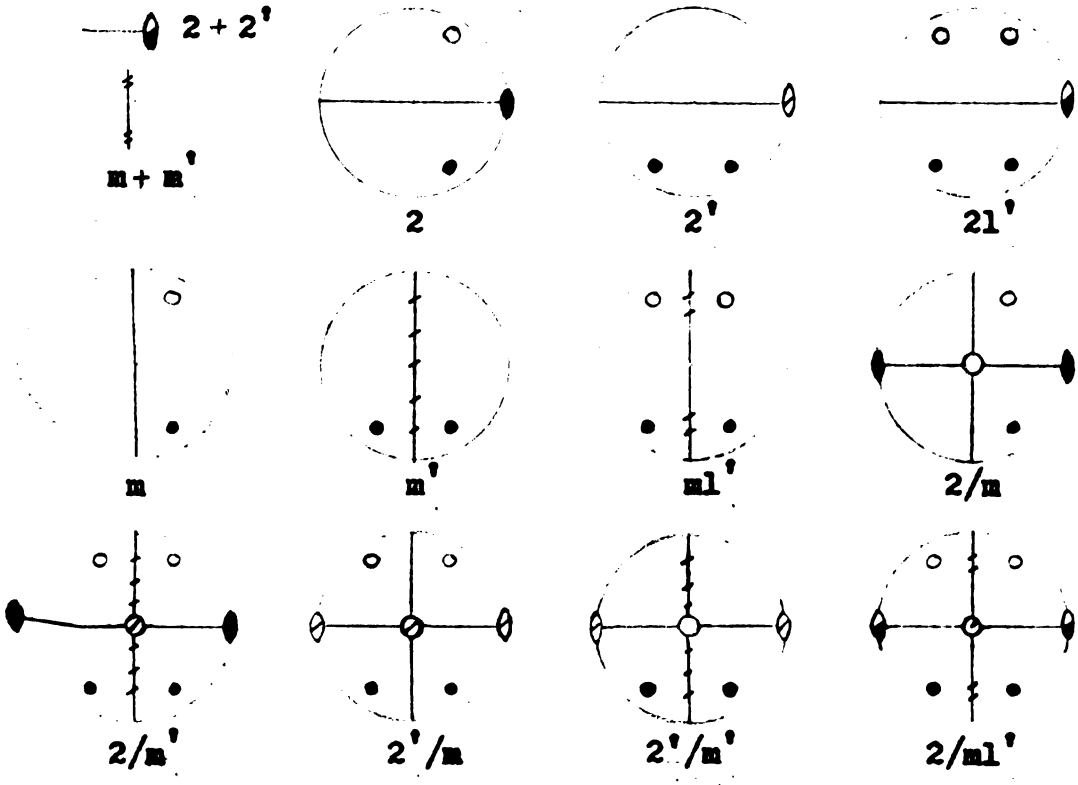


Fig. 11. Symmetry of an Axial Vector under the Monoclinic Heesch Point Groups



The symmetry operations comprising each of the triclinic point groups have been listed in Table 2. Those for the monoclinic system are listed in Table 9.

Table 9. Monoclinic Heesch Point Groups

Point Group (in Belov notation)	Symmetry operations or group elements
2	2,E
2'	2',E
21'	2,2',E,E'
m	m,E
m'	m',E
ml'	m,m',E,E'
2/m	2,m,i,E
2/m'	2,m',i',E
2'/m	2',m,i',E
2'/m'	2',m',i,E
2/ml'	2,m,i,E,2',m',i',E'

X-Ray Structure

The chemical space group of azurite is $P2_1/c$ at room temperature.[24] The unit cell dimensions are: $a_o = 5.00$, $b_o = 5.85$, $c_o = 10.35$Å, $\beta = 92°20'$. The copper ions may be divided in two sets. In the first set are the ions which occupy the special position

$$0,0,0;0,\tfrac{1}{2},\tfrac{1}{2}.$$

24. G. Gattow und J. Zemann, Acta Cryst. 11, 866 (1958).

The second set occupy the general position

$$x,y,z;\ \bar{x},\bar{y},\bar{z};\ \tfrac{1}{2}+y,\ \tfrac{1}{2}-z;\ x,\ \tfrac{1}{2}-y,\ \tfrac{1}{2}+z,$$

where $x = 0.252$, $y = 0.495$ and $z = 0.085$. There are also four hydroxyl radicals in general position.

Point Group Selection

There are two possibilities to consider at 1.6°K.

1. The symmetry of the atomic positions remains $P2_1/c$.
2. Statement number 1. is false.

If atomic positions are altered so that the x-ray symmetry is no longer $P2_1/c$ in a crystal with as complicated a structure as azurite, it is almost certain that the symmetry change would result in a triclinic crystal. If the x-ray symmetry is triclinic at 1.6°K, then one of the triclinic Shubnikov space groups must represent the symmetry of the magnetic cell. Then this group must correspond to one of the triclinic Heesch point groups in Fig. 10. However, none of the triclinic point groups of Fig. 10 have the observed axial point group symmetry shown in Fig. 8. Therefore, we shall assume in the future that the x-ray symmetry of azurite at 1.6°K is $P2_1/c$. There exist however, four other possibilities. Before proceeding further these will be discussed.

1. If the x-ray symmetry at 1.6°K is triclinic, it would still be possible to observe the local field pattern shown in Fig. 7., as the point groups $1', \bar{1}'$ and $\bar{1}1'$ in Fig. 10 permit the

observed symmetry provided that vectors 1 and 2 and 5 and 6 of Fig. 7 are unrelated to each other by any symmetry operation. This would imply that the observed symmetry of orientation which for example seems to relate vectors 1, 2, 3 and 4 is accidental. This possibility is unlikely especially in view of the fact that the magnitudes of the vectors 1, 2, 3 and 4 are the same.

2. Suppose the x-ray symmetry at 1.6°K is a monoclinic space group other than $P2_1$, Pc or $P2_1/c$. Again, this would require a considerable rearrangement of ions and therefore lead almost certainly to triclinic symmetry.
3. If the x-ray symmetry at 1.6°K belongs to some system other than triclinic or monoclinic[25], then the Heesch point group might also be one of higher symmetry than those in the monoclinic system. An investigation of all of the point groups of these higher symmetry systems shows none which predict the observed axial vector symmetry.
4. In the event that the x-ray symmetry is $P2_1$, or Pc at 1.6°K, none of the arguments to follow need be altered. The only change would appear

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[25]. The possibility, although unlikely, exists: see L. D. Landau and E. M. Lifshitz, Statistical Physics (Addison-Wesley Publishing Company, Inc., Massachusetts, 1958) p.433.

in the final conclusion. If, for example, the x-ray symmetry at 1.6°K were $P2_1$, then instead of the four Shubnikov groups found in Table 10 as representing the possible magnetic space group symmetries, P_a2_1 could be immediately selected as the only possible antiferromagnetic symmetry group. That is, it would be the only one of the four groups which would have the correct x-ray symmetry.

In view of the previous remarks, the point group in the antiferromagnetic state must satisfy the following conditions:

1. The point group must transform an arbitrary axial vector in the same way as is permitted by the resonance pattern. (Fig. 8 for azurite).
2. The ordinary crystallographic point group obtained by replacing all antioperations of the point group by their corresponding ordinary operations must be either a proper or improper subgroup of the ordinary crystallographic point group of the crystal. For azurite, this is 2/m.

From Fig. 11 it appears that the only point groups which satisfy these requirements are $2'/m$, $2/m'$, $2/ml'$, $2l'$ and ml'.

Space-Group Requirements

If the crystal structure and resonance data (previously described for azurite) are available, then one may proceed

to select as possible antiferromagnetic space groups those groups in Table 6 which satisfy the following requirements.

1. The operations of the Shubnikov space group must leave unaltered the positions of the ions as determined by the x-ray data. This implies that if a symmetry operation of the Shubnikov group transforms the ion position $\vec{r}$ into $\vec{R}$, then the chemical space group must contain a corresponding symmetry operation which will transform $\vec{r}$ into $\vec{R}$. The converse <u>is not</u> true and therefore there may exist pairs of ions whose positions are related by symmetry operations of the chemical space group but which are not related by a symmetry operation of the Shubnikov group.
2. The Shubnikov space group must have as its point group one of the possible point groups predicted by the data. For azurite, this is one of the five point groups found above.
3. The Shubnikov group must permit a magnetic unit cell which contains the same number of protons with different local magnetic fields as there are resonance lines in the nuclear magnetic resonance pattern. For azurite, this number is eight.
4. A magnetic ion may not occupy an anticenter. An anti-inversion moves an axial vector through

the anticenter and then reverses its sense. Hence, the magnetic moment of an ion located at an anticenter is zero.

Space-Group Selection

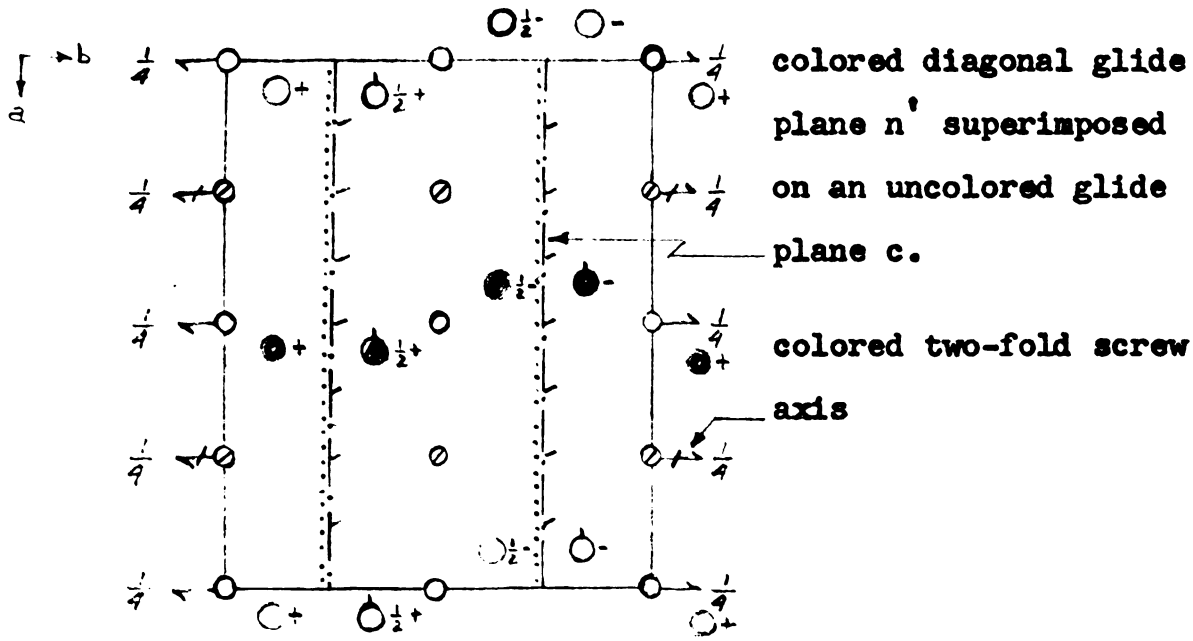
The left-hand column in Table 10 consists of all those monoclinic groups in Table 6 which satisfy the previously discussed requirement number 1. An asterisk to the right of a group under one of the columns indicates that that particular requirement number which heads the column is not satisfied by the group. In the last column at the right, the corresponding point groups are listed.

Table 10. Space Group Selection

Shubnikov Space Group	Requirement 2	3	4	Point Group
P_a2_1/c		*		$2/ml'$
$P2_1'/c'$	*	*		$2'/m'$
$P2_1/c'$		*	*	$2/m'$
$P2_1'/c$		*	*	$2'/m$
$P2_1/c$	*	*		$2/m$
C_ac				ml'
P_bc				ml'
P_ac				ml'
Pc'	*	*		m'
Pc	*	*		m
P_a2_1				$21'$
$P2_1'$	*	*		$2'$
$P2_1$	*	*		2

Consider Fig. 17 page 53. Disregarding for the time being the numbers in the circles, it may be seen from the x-ray data that the circles represent the positions of the copper ions in two chemical cells placed next to each other along the x direction where the x,y and z axes of Fig. 17 coincide with the a,b and c crystallographic axes in the x-ray section. Let us now investigate the group P_a2_1/c in Table 10. Fig. 12 is a diagram of the group where the solid rectangle represents the outline of the projection of the double chemical cell of Fig. 17 in the x,y plane. A double chemical cell is needed for P_a2_1/c since the group contains an antitranslation in the a direction. The unit cell of P_a2_1/c is therefore just twice the volume of the chemical cell. The unit cell of this group therefore contains eight protons. However, as may be seen from the

Fig. 12. Diagram of P_a2_1/c.



following they do not possess different local fields. Suppose the components of the local magnetic field at one proton located at (x,y,z) is H_x,H_y,H_z. The anticenter at $(\frac{1}{4},\frac{1}{2},\frac{1}{2})$ in the magnetic cell implies that the proton at $(\frac{1}{2}-x,\bar{y},\bar{z})$ will experience a local field the components of which are $\bar{H}_x,\bar{H}_y$ and $\bar{H}_z$ where the bar indicates a negative quantity. The two protons as well as the local field vectors are translated to $(x+\frac{1}{2},y,z)$ and $(\bar{x},\bar{y},\bar{z})$ respectively by the antitranslation in the a direction. The local field components at these positions are then $\bar{H}_x,\bar{H}_y,\bar{H}_z$ and H_x,H_y,H_z. Thus only two of these four protons experience different local magnetic fields. A similar argument applied to the remaining four protons leads to a similar conclusion, indicating that there are in all only four proton positions at which there are different local fields in the unit cell of P_a2_1/c.

The group P_ac, the diagram of which is shown in Fig. 13, also contains an antitranslation in the a direction.* Therefore, the magnetic unit cell of this group contains eight protons. These may be divided into two sets of four each in such a way as to make those in one set completely independent of those in the other set as far as the operations of the group P_ac are concerned. Let the components of the local field vector at the proton position (x,y,z) in one set

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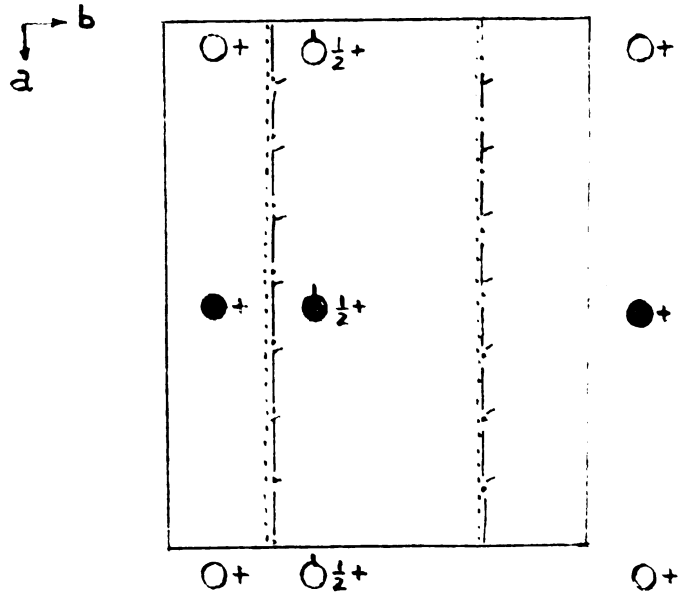
*In the diagrams of the space groups P_ac, P_a2_1, P_bc and C_ac to follow, as well as the group P_a2_1/c, the a, b, and c crystallographic axes coincide with the x,y and z cell axes with one exception. In the diagram of the group P_ac, the c axis is directed from cell coordinates (0,0,0) to $(\frac{1}{2},0,1)$.

Fig. 13. Diagram of P_ac.



be H_x,H_y, and H_z and those of a proton in the other set at (x',y',z') be $H_{x'}$, $H_{y'}$, and $H_{z'}$ where the positions (x,y,z) and (x',y',z') are related by the operations of the space group $P2_1/c$ but are unrelated by those of P_ac. The existence of eight different local fields is predicted by the group operations as shown in Table 11 where c,n, and t_a represent a glide reflection (reflection followed by a translation of half the length of the magnetic cell in the c direction), a diagonal glide reflection and a translation in the a direction respectively.

Similar magnetic field transformation tables may be constructed for the groups P_a2_1 and P_bc. Their diagrams are shown in Figs. 14 and 15.

Table 11. Magnetic Field Transformations under $P_a c$

E	c	n'	t_a'
x,y,z	$x,\frac{1}{2} - y,z + \frac{1}{2}$	$x + \frac{1}{2},\frac{1}{2} - y,z + \frac{1}{2}$	$x + \frac{1}{2},y,z$
H_x	$\bar{H}_x$	H_x	$\bar{H}_x$
H_y	H_y	$\bar{H}_y$	$\bar{H}_y$
H_z	$\bar{H}_z$	H_z	$\bar{H}_z$
x',y',z'	$x',\frac{1}{2} - y',z' + \frac{1}{2}$	$x' + \frac{1}{2},\frac{1}{2} - y',z' + \frac{1}{2}$	$x' + \frac{1}{2},y',z'$
H_x'	$\bar{H}_x'$	H_x'	$\bar{H}_x'$
H_y'	H_y'	$\bar{H}_y'$	$\bar{H}_y'$
H_z'	$\bar{H}_z'$	H_z'	$\bar{H}_z'$

Fig. 14. Diagram of $P_a 2_1$.

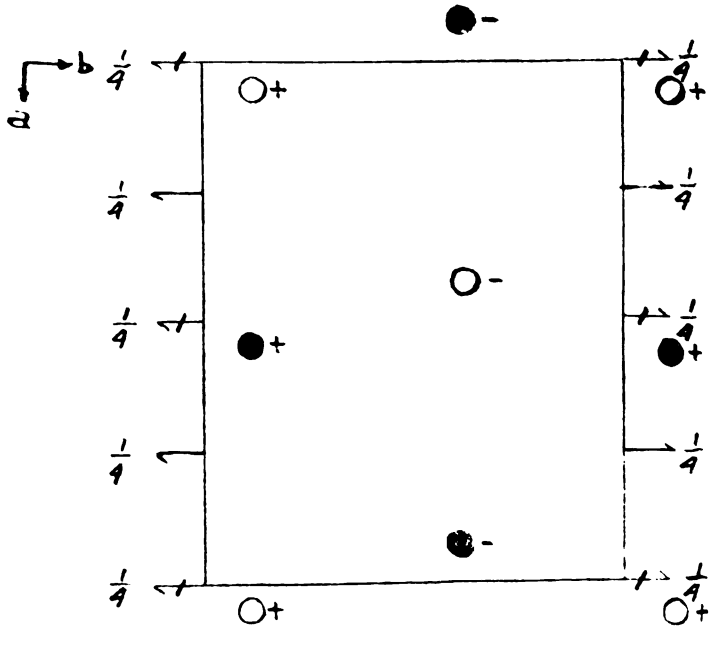
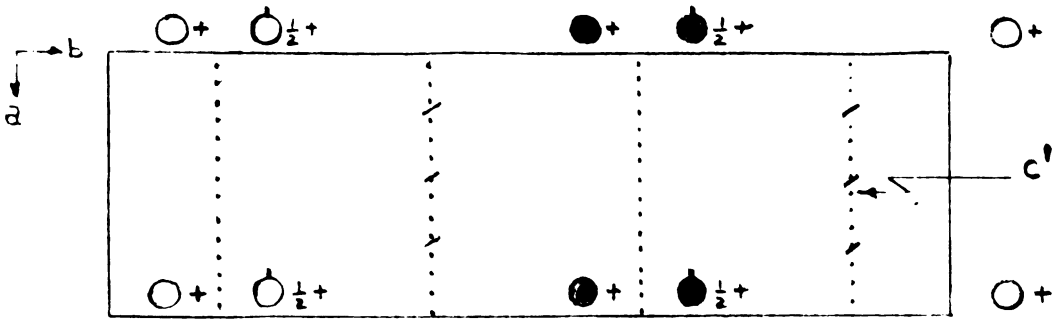


Fig. 15. Diagram of $P_b c$



For brevity, only the local fields at the proton positions belonging to one of the two sets of protons are shown in Tables 12 and 13. The other set is obvious as in the case of $P_a c$.

Table 12. Magnetic Field Transformations under $P_a 2_1$

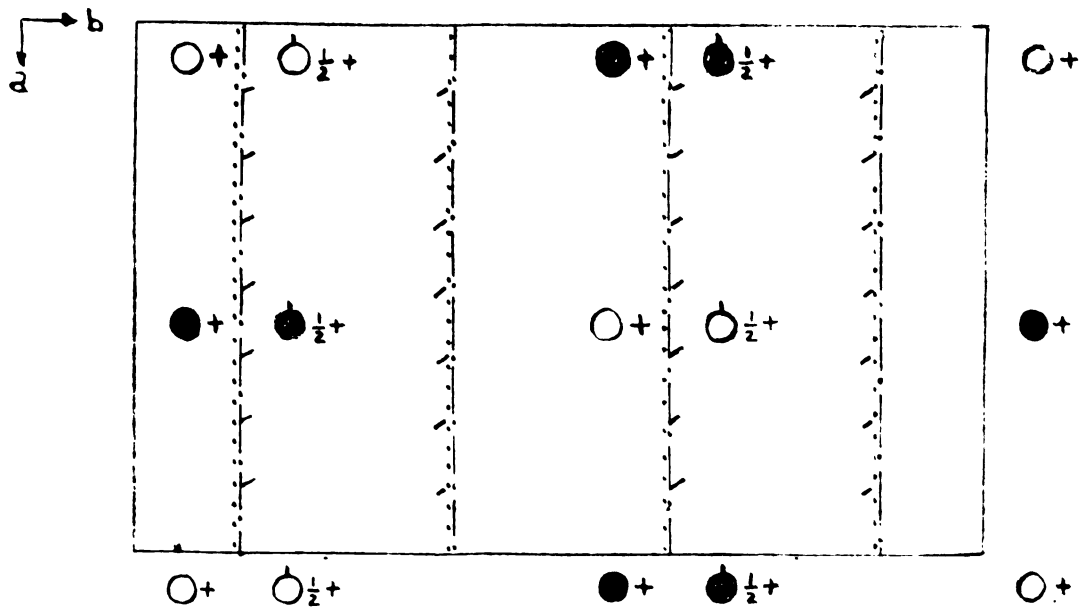
E	2_1	$2_1'$	t_a'
x,y,z	$\frac{1}{2} - x,y + \frac{1}{2},\frac{1}{2} - z$	$1 - x,y + \frac{1}{2},\frac{1}{2} - z$	$x + \frac{1}{2},y,z$
H_x	$\bar{H}_x$	H_x	$\bar{H}_x$
H_y	H_y	$\bar{H}_y$	$\bar{H}_y$
H_z	$\bar{H}_z$	H_z	$\bar{H}_z$

Table 13. Magnetic Field Transformations under $P_b c$

E	c	c'	t_b'
x,y,z	$x,\frac{1}{4} - y,z + \frac{1}{2}$	$x,\frac{3}{4} - y,z + \frac{1}{2}$	$x,y + \frac{1}{2},z$
H_x	$\bar{H}_x$	H_x	$\bar{H}_x$
H_y	H_y	$\bar{H}_y$	$\bar{H}_y$
H_z	$\bar{H}_z$	H_z	$\bar{H}_z$

The antitranslation in both the a and b crystallographic directions in the group $C_a c$ leads to a unit magnetic cell four times the volume of the chemical cell. The diagram is shown in Fig. 16.

Fig. 16. Diagram of $C_a c$



The sixteen protons in this magnetic cell may be divided into two sets of eight each, again in such a way as to make those in one set unrelated by the operations of $C_a c$ to those in the other set. As above, only the local fields at the proton positions in one set are shown in Table 14.

Table 14. Magnetic Field Transformations under $C_a c$

E	c	c'	n
x,y,z	$x,\frac{1}{4}-y,z+\frac{1}{2}$	$x,\frac{3}{4}-y,z+\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4}-y,z+\frac{1}{2}$
H_x	$\bar{H}_x$	H_x	$\bar{H}_x$
H_y	H_y	$\bar{H}_y$	H_y
H_z	$\bar{H}_z$	H_z	$\bar{H}_z$
n'	**t_b'**	**t_a'**	**t_a't_b'**
$x+\frac{1}{2},\frac{1}{4}-y,z+\frac{1}{2}$	$x,y+\frac{1}{2},z$	$x+\frac{1}{2},y,z$	$x+\frac{1}{2},y+\frac{1}{2},z$
H_x	$\bar{H}_x$	$\bar{H}_x$	H_x
$\bar{H}_y$	$\bar{H}_y$	$\bar{H}_y$	H_y
H_z	$\bar{H}_z$	$\bar{H}_z$	H_z

Possible Magnetic Structures

Two possible magnetic structures with the symmetry of the groups $P_a c$ and $P_a 2_1$ are shown in Figs. 17 and 18 respectively. Tables 15 and 16 accompany the figures. Magnetic structures for the two remaining groups[26] $P_b c$ and $C_a c$ are illustrated in Tables 17 and 18. The first number in the symbols in the left-hand column of each of the tables 15, 16, 17, and 18 designates one of the four magnetic moments which belong to that particular family of ions which are all connected by the group operations. The second number in the same symbol indicates to which one of the three families (1,2, or 3) the ion belongs. The copper ions in special

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[26]. The structure suggested by W. Van der Lugt and N. J. Poulis (Physica 25, 1313(1959)) is permitted by the group C_{ac}.

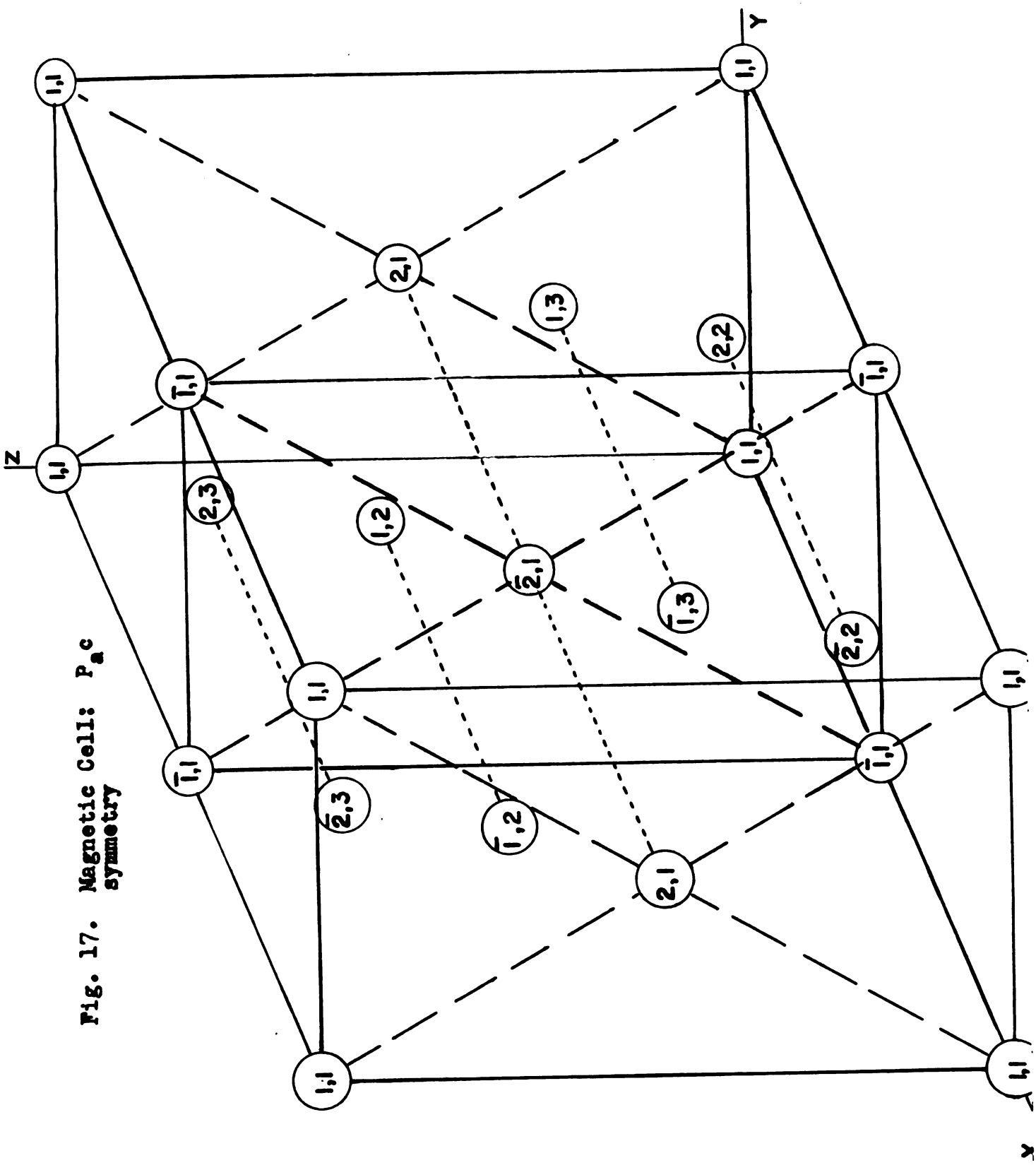

Fig. 17. Magnetic Cell: P_a^c symmetry

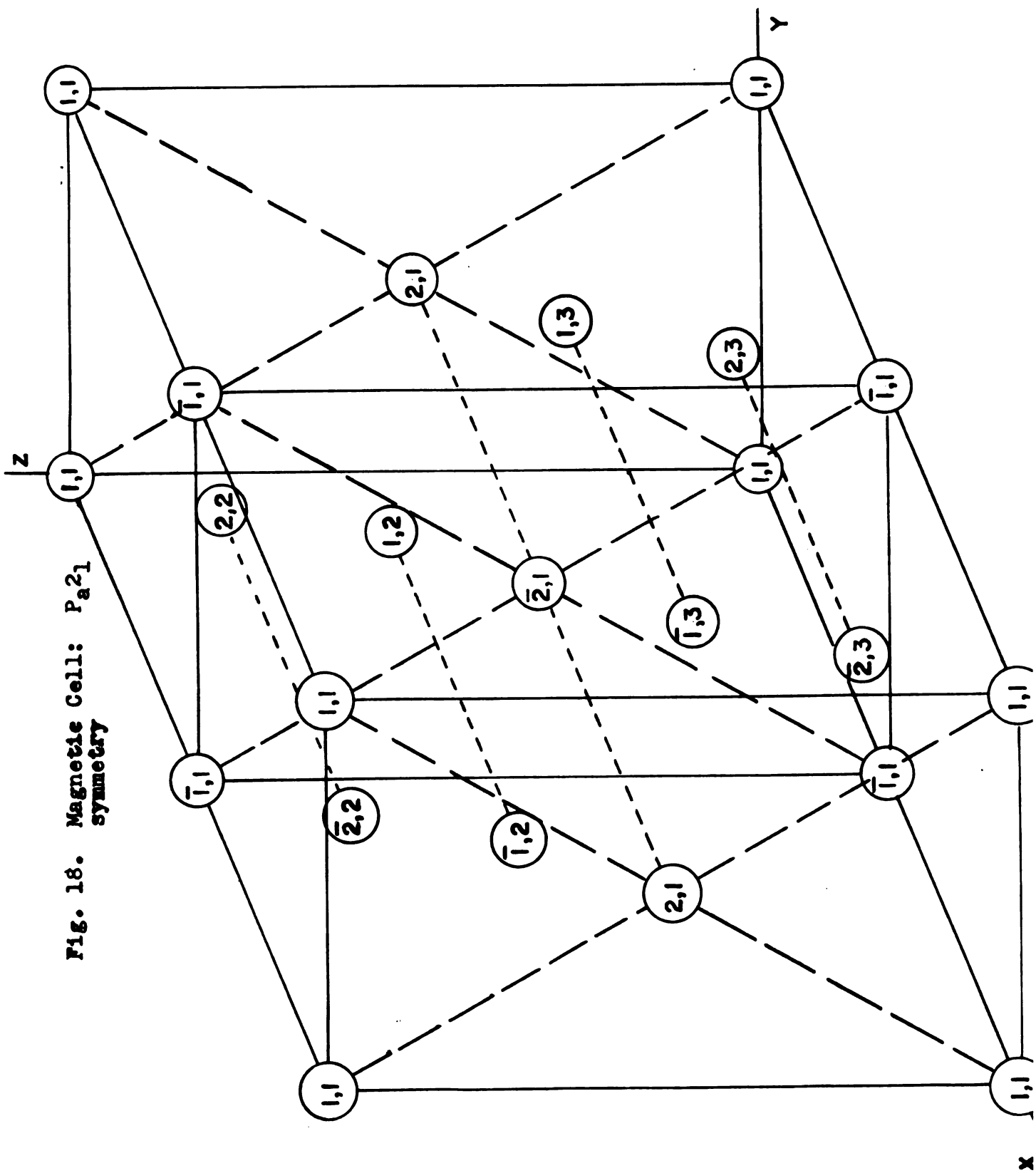

Fig. 18. Magnetic Cell: P_a2_1 symmetry

Table 15. Magnetic Structure: P_ac symmetry

Numbers in symbol at copper ion position	Ion position (x,y,z) in magnetic cell	Magnetic Moment Components	Ion in set number*)
1,1	0,0,0	u_{1x}, u_{1y}, u_{1z}	1
$\bar{1}$,1	$\frac{1}{2}$,0,0	$\bar{u}_{1x}, \bar{u}_{1y}, \bar{u}_{1z}$	1
2,1	0,$\frac{1}{2}$,$\frac{1}{2}$	$u_{1x}, \bar{u}_{1y}, u_{1z}$	1
$\bar{2}$,1	$\frac{1}{2}$,$\frac{1}{2}$,$\frac{1}{2}$	$\bar{u}_{1x}, u_{1y}, \bar{u}_{1z}$	1
1,2	.126,.005,.585	u_{2x}, u_{2y}, u_{2z}	2
$\bar{1}$,2	.626,.005,.585	$\bar{u}_{2x}, \bar{u}_{2y}, \bar{u}_{2z}$	2
2,2	.126,.495,.085	$u_{2x}, \bar{u}_{2y}, u_{2z}$	2
$\bar{2}$,2	.626,.495,.085	$\bar{u}_{2x}, u_{2y}, \bar{u}_{2z}$	2
1.3	.374,.995,.415	u_{3x}, u_{3y}, u_{3z}	2
$\bar{1}$,3	.874,.995,.415	$\bar{u}_{3x}, \bar{u}_{3y}, \bar{u}_{3z}$	2
2,3	.374,.505,.915	$u_{3x}, \bar{u}_{3y}, u_{3z}$	2
$\bar{2}$,3	.874,.505,.915	$\bar{u}_{3x}, u_{3y}, \bar{u}_{3z}$	2

*) See section on x-ray data

position (set number 1 in the right-hand column of the above four tables) are not connected by the operations of the group, for which the particular table is constructed, to those in general position (set number 2).

If every copper ion which is linked to another copper ion through a common oxygen ion is coupled antiferromagnetically by a super-exchange mechanism to the other copper ion, the resulting magnetic structure forbids an anti-translation

Table 16. Magnetic Structure: P_a2_1 symmetry

Numbers in symbol at copper ion position	Ion position (x,y,z) in magnetic cell	Magnetic Moment Components	Ion in set number
1,1	0,0,0	u_{1x}, u_{1y}, u_{1z}	1
$\bar{1}$,1	½,0,0	$\bar{u}_{1x}, \bar{u}_{1y}, \bar{u}_{1z}$	1
2,1	0,½,½	$u_{1x}, \bar{u}_{1y}, u_{1z}$	1
$\bar{2}$,1	½,½,½	$\bar{u}_{1x}, u_{1y}, \bar{u}_{1z}$	1
1,2	.126,.005,.585	u_{2x}, u_{2y}, u_{2z}	2
$\bar{1}$,2	.626,.005,.585	$\bar{u}_{2x}, \bar{u}_{2y}, \bar{u}_{2z}$	2
2,2	.374,.505,.915	$\bar{u}_{2x}, u_{2y}, \bar{u}_{2z}$	2
$\bar{2}$,2	.874,.505,.915	$u_{2x}, \bar{u}_{2y}, u_{2z}$	2
1,3	.374,.995,.415	u_{3x}, u_{3y}, u_{3z}	2
$\bar{1}$,3	.874,.995,.415	$\bar{u}_{3x}, \bar{u}_{3y}, \bar{u}_{3z}$	2
2,3	.126,.495,.085	$\bar{u}_{3x}, u_{3y}, \bar{u}_{3z}$	2
$\bar{2}$,3	.626,.495,.085	$u_{3x}, \bar{u}_{3y}, u_{3z}$	2

in the b direction. In such a case, the groups P_ac and P_a2_1 are the only possibilities.

It should be noted that except for the fact that they are not zero no use has been made in the above analysis of the magnitudes of the local field vectors listed in Table 8. In principle it may be possible to obtain a complete description of the magnetic structure by combining the known local fields in the antiferromagnetic state with the positions of the protons obtained from proton resonance in the

Table 17. Magnetic Structure: P_bc symmetry

Numbers in symbol at copper ion position	Ion position (x,y,z) in magnetic cell	Magnetic Moment Components	Ion in set number
1,1	0,0,0	u_{1x}, u_{1y}, u_{1z}	1
$\bar{1}$,1	0,½,0	$\bar{u}_{1x}, \bar{u}_{1y}, \bar{u}_{1z}$	1
2,1	0,¼,¼	$\bar{u}_{1x}, u_{1y}, \bar{u}_{1z}$	1
$\bar{2}$,1	0,¾,¼	$u_{1x}, \bar{u}_{1y}, u_{1z}$	1
1,2	.252,.0025,.585	u_{2x}, u_{2y}, u_{2z}	2
$\bar{1}$,2	.252,.5025,.585	$\bar{u}_{2x}, \bar{u}_{2y}, \bar{u}_{2z}$	2
2,2	.252,.2475,.085	$\bar{u}_{2x}, u_{2y}, \bar{u}_{2z}$	2
$\bar{2}$,2	.252,.7475,.085	$u_{2x}, \bar{u}_{2y}, u_{2z}$	2
1,3	.748,.2525,.915	u_{3x}, u_{3y}, u_{3z}	2
$\bar{1}$,3	.748,.7525,.915	$\bar{u}_{3x}, \bar{u}_{3y}, \bar{u}_{3z}$	2
2,3	.748,.4975,.415	$u_{3x}, \bar{u}_{3y}, u_{3z}$	2
$\bar{2}$,3	.748,.9975,.415	$\bar{u}_{3x}, u_{3y}, \bar{u}_{3z}$	2

paramagnetic phase and the known crystal structure. However, the work of Poulis et al. on $CuCl_2 \cdot 2H_2O$ has clearly indicated that this program is extremely difficult if not impossible.

Table 18. Magnetic Structure: $C_a c$ symmetry

Numbers in symbol at copper ion position	Ion position (x,y,z) in magnetic cell	Magnetic moment components	Ion in set number
1,1	$(0,0,0),(\frac{1}{2},\frac{1}{2},0)$	u_{1x},u_{1y},u_{1z}	1
$\bar{1}$,1	$(\frac{1}{2},0,0),(0,\frac{1}{2},0)$	$\bar{u}_{1x},\bar{u}_{1y},\bar{u}_{1z}$	1
2,1	$(0,\frac{1}{4},\frac{1}{2}),(\frac{1}{2},\frac{3}{4},\frac{1}{2})$	$\bar{u}_{1x},u_{1y},\bar{u}_{1z}$	1
$\bar{2}$,1	$(0,\frac{3}{4},\frac{1}{2}),(\frac{1}{2},\frac{1}{4},\frac{1}{2})$	$u_{1x},\bar{u}_{1y},u_{1z}$	1
1,2	(.126,.0025,.585),(.626,.5025,.585)	u_{2x},u_{2y},u_{2z}	2
$\bar{1}$,2	(.125,.5025,.585),(.626,.0025,.585)	$\bar{u}_{2x},\bar{u}_{2y},\bar{u}_{2z}$	2
2,2	(.126,.2475,.085),(.626,.7475,.085)	$\bar{u}_{2x},u_{2y},\bar{u}_{2z}$	2
$\bar{2}$,2	(.126,.7475,.085),(.626,.2475,.085)	$u_{2x},\bar{u}_{2y},u_{2z}$	2
1,3	(.374,.2525,.915),(.874,.7525,.915)	u_{3x},u_{3y},u_{3z}	2
$\bar{1}$,3	(.374,.7525,.915),(.874,.2525,.915)	$\bar{u}_{3x},\bar{u}_{3y},\bar{u}_{3z}$	2
2,3	(.374,.4975,.415),(.874,.9975,.415)	$u_{3x},\bar{u}_{3y},u_{3z}$	2
$\bar{2}$,3	(.374,.9975,.415),(.874,.4975,.415)	$\bar{u}_{3x},u_{3y},\bar{u}_{3z}$	2

Section III

Twinning by Merohedry and Reticular Merohedry

Introduction

Two identical crystals (or individuals) are said to be in twin relation to each other if they are joined together in some way such that the pair possesses an element of macroscopic symmetry which is not a symmetry element of either individual. This element of macroscopic symmetry is the same as that dealt with in crystal morphology. A plane of symmetry which relates two twinned individuals to each other (twin plane) must be parallel to a lattice plane in both individuals. A twin axis must be parallel to a lattice row common to both individuals.

With rare exceptions, all known twins can be described in one of four ways (known as Friedel's rules of twinning.)[27]

1. The individuals of the twin are related by a twin symmetry element which is an element of symmetry of the lattice of each individual but which is not a symmetry element of the crystal (i.e., either individual). This type of twinning is called twinning by merohedry.*

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[27] See the review by R. W. Cahn, Advances in Phys. 3, 363 (1954).

* The term merohedry, of Greek origin, implies that each individual of the twin has fewer faces than it would have if it had the full symmetry of its lattice.

2. The individuals of the twin are related by a twin symmetry element which is an element of symmetry of what is called a coincidence lattice but which is not a symmetry element of the crystal. The coincidence lattice extends from one individual to the other without modification but consists of only some of the lattice points of each. This type of twinning is called twinning by reticular (or lattice) merohedry.
3. The individuals of the twin are related by a twin symmetry element which is <u>almost</u> a symmetry element of the lattice (i.e., a pseudo-symmetry element of the lattice). This method of twinning is therefore just an extension of the first method and is called twinning by pseudo-merohedry.
4. The individuals of the twin are related by a twin symmetry element which is <u>almost</u> an element of symmetry of a coincidence lattice. This extension of the second method is called twinning by pseudo-reticular merohedry.

The formalism of the Heesch groups has only recently been employed by Curien and Le Corre[28] to describe all of the possible merohedry and reticular merohedry twin relations in crystals the symmetry of which is completely described by

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28. H. Curien, and Y. Le Corre, op. cit.

the position of the ions. These relations are called twin groups.

Although twinning in the antiferromagnetic crystal NiO has been observed*, so far as is known to the author no one has yet described the possible merohedry and reticular merohedry twin relations in antiferromagnetic crystals. These twin groups are constructed and listed in this section. A total of 177 merohedry twin groups are described; of these, 35 are the same as the 35 merohedry twin groups found by Curien and Le Corre while the remaining 142 groups are new. In addition, 51 reticular merohedry twin groups are listed; of these, 11 are the same as the 11 reticular merohedry twin groups found by Curien and Le Corre while the remaining 40 groups are new.

Twinning by Merohedry

a. Ordinary Lattices

If the symmetry of a crystal is lower than the symmetry of its lattice, twinning by merohedry is possible. This is because there are then various possible orientations of the atoms of the crystal relative to its lattice. A possible twin operation is an operation which relates one of the possible orientations of the atoms to another. These operations are the point group symmetry operations of the lattice which are not contained in the point group of the crystal. But

*Discussed at the end of this section

what are the point group symmetry operations of the lattice? In ordinary crystallography, these operations comprise the highest point group symmetry possible for the particular symmetry system to which the lattice belongs (This is called the holohedral point group.). For example, for the monoclinic lattices, the holohedral point group is 2/m. For our purposes, it is helpful to think of the holohedral point group as resulting from the fact that the symmetry of the monoclinic lattices permit the simultaneous existence of a two-fold axis (or two-fold screw axis) and a plane (or glide plane). These two operations also imply a center of symmetry and hence the group 2/m contains 4 elements. Consider now a crystal which has point symmetry 2. According to the above, it is therefore possible from the standpoint of symmetry for the crystal to twin by merohedry by either a twin plane or an inversion center (it will later be shown that these two are equivalent in this case). Curien and Le Corre express this fact by using the Heesch group $2/m'$ which they call a twin group. The twin group therefore expresses the point symmetry of the crystal (2) and also identifies the equivalent twin operations (m' and $1'$) through the use of a prime (see Table 9). In the next two paragraphs the notation in Section II for the Heesch groups will be used to express twin groups. However, a prime will only denote a colored operation which may or may not be a twin operation. A twin operation will be those operations not contained in the point group of the crystal but which are included in the "holohedral"

point group. In all work which follows the next two paragraphs, an asterisk will be used to explicitly indicate twin operations and the twin group notation will be changed. For example, Curien and Le Corre's twin group $2/m'$ above will be denoted by $2;P_y^*$.

Suppose that the point group of a crystal under consideration is $2'$. The lattice of this crystal is the same as the previous crystal, i.e., an ordinary uncolored lattice. However, as the list of Shubnikov groups show, the uncolored lattices of the monoclinic system permit the simultaneous existence of combinations of colored axes with colored and uncolored symmetry planes which result in two "holohedral" point groups as far as the crystal with point group $2'$ is concerned. These are $2'/m$ and $2'/m'$. These two groups imply two possible twin groups and therefore two possible distinct twins. The equivalent twin operations implied by the first group ($2'/m$) are an uncolored mirror plane and a colored inversion center, while those implied by the second group are a colored mirror plane and an uncolored center.

Let us return to the example where the crystal has point symmetry 2. If the crystal is a type for which its symmetry is completely expressed by the position of its ions, then the only twin group which exists is that found by Curien and Le Corre, discussed above. If the crystal possesses some other characteristic (such as magnetic moments) so that it belongs to a general category of crystals (such as antiferromagnetic crystals) the symmetry of which can be described by

the Shubnikov group theory, then there exists the possibility of colored twin operations even though the point group of the crystal is uncolored. Proceeding then, in the same way as in the case of point symmetry 2' (where the possibility of colored twin operations must obviously be considered) leads to another "holohedral" point group 2/m'. This twin group implies that the crystal can twin by a colored plane or equivalently by a colored inversion center.

It is therefore evident that the point symmetry of the lattice must be modified as described above in extending the idea of twinning to types of crystals subject to the Shubnikov theory whose space groups are based on ordinary lattices.

b. Black-White Lattices

For twinning in black-white lattices there is always only one holohedral point group. This group is just the gray Heesch group which may be constructed from the ordinary (or uncolored) holohedral Heesch group by introducing the element E'. For example, 2/m→2/ml'.

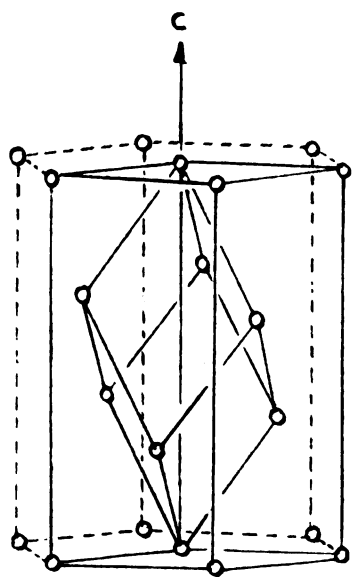
Twinning by Reticular Merohedry

When twinning by reticular merohedry takes place, the lattices of the two members of a twin are not parallel in orientation. There exists, however, what is called a coincidence lattice which consists of some of the lattice points of both individuals and continues from one individual to the other without modification. The remarks made above concerning the "holohedral" point groups of uncolored (or ordinary) lattices and the holohedral point group of black-white

lattices are also true for uncolored and black-white coincidence lattices.

a. Ordinary Lattices. A coincidence lattice may be defined for rhombohedral and cubic crystals. This coincidence lattice consists of some of the lattice points of the rhombohedral lattice for a rhombohedral crystal and some of the lattice points of the cubic lattice for a cubic crystal. For rhombohedral crystals, the coincidence lattice is only those points of the rhombohedral lattice which generate those lattice points described by the symmetry of a hexagonal prism. The hexagonal prism and the rhombohedral lattice R is shown on page 20 in the "The International Tables for X-Ray Crystallography" and redrawn for convenience in Fig. 19.

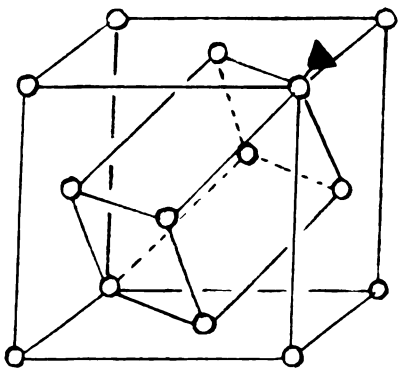
Fig. 19. Hexagonal Prism and Rhombohedral Lattice R.



The hexagonal prism is just a multiple of the C lattice of the hexagonal system in Fig. 5. Hence, possible reticular merohedry twin operations for rhombohedral crystals will be point group operations contained in the hexagonal system which are not symmetry operations of the rhombohedral crystal.

For cubic crystals, the coincidence lattice consists of only those points of the cubic lattice which generate the lattice points described by the symmetry of a hexagonal prism. This hexagonal prism is the same as the one generated for rhombohedral crystals and arises in exactly the same way, i.e., from a rhombohedral lattice. The origin of the rhombohedral lattice in cubic crystals is clear when it is remembered that cubic lattices are just special cases of rhombohedral lattices. As an example, consider the face-centered cubic F lattice. It may also be described by a rhombohedral primitive cell shown in Fig. 20.

Fig. 20. The Rhombohedral Primitive Cell of the the Face-Centered Cubic F Lattice



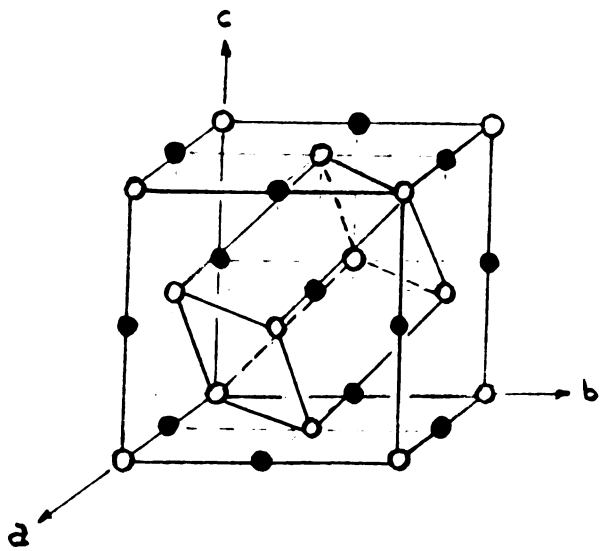
The operations available for possible twinning by reticular merohedry in cubic crystals are therefore those operations of the hexagonal system which are not symmetry operations of the cubic crystal.

Since there are four space diagonals of a cube, the rhombohedral primitive cell can be oriented in four ways. This implies four possible orientations of the hexagonal lattice with respect to the cube. Then a possible reticular merohedry twin operation can be oriented in four possible directions. The six-fold rotation axis for example can have the direction of any one of the four space diagonals of the cube.

b. Black-White Lattices. If the rhombohedral lattice in Fig. 19 is body centered with a black lattice point, it becomes the black-white rhombohedral lattice R_I in Fig. 5. The hexagonal prism then has a colored translation in the c direction and is just a multiple of the C_c lattice of the hexagonal system in Fig. 5. This implies that the coincidence lattice for rhombohedral crystals with lattice R_I consists of those points of the rhombohedral lattice R_I which generate the lattice points of a hexagonal prism with a colored translation in the c direction. The possible operations of reticular merohedry twinning for crystals with lattice R_I are then those point group operations compatible with the symmetry of the black-white hexagon which are not point symmetry operations of the rhombohedral crystal. The holohedral point group of the black-white hexagon is $6/mml'$.

As mentioned above, the lattice P of the cubic system is a special case of the lattice R of the rhombohedral system. Similarly, the lattice P_I of the cubic system is a special case of the lattice R_I. The only other black-white lattice in the cubic system, F_s, is also a special case of R_I. This is shown in Fig. 21.

Fig. 21. The Rhombohedral Primitive Cell R_I of the Face-Centered Cubic Lattice F_s



For cubic crystals with black-white lattices, the coincidence lattice is therefore the same as the coincidence lattice for rhombohedral crystals with lattice R_I. The possible reticular merohedry twin operations are therefore those point group operations compatible with the symmetry of the black-white hexagon which are not point symmetry operations of the cubic crystal.

Merohedry Twin Notation

Let a twin operation be denoted by q^*. This operation may be thought of in the following way. The operation q is the operation which transforms one individual of the twin at position #1 to the other individual at position #2. The * then colors the individual at position #2 black while the other individual is left uncolored. If t is this coloring operation we may write $q^* = tq$. If the coloring takes place before the operation q, the result is still the same, i.e., $q^* = qt$, or t commutes with q. Since there are only two colors, $t^2 = E$. Thus t has the same mathematical properties as the reversal operator (see Section II).

A twin group g_t is defined as a set of elements of the general type $\{p_i, q_i^*\}$ satisfying the group properties with the following structure: the set $\{p_i\}$ is a subgroup of index two of g_t and $\{p_i\} \equiv H$ where H is the Heesch group of each of the two individuals of the twin. Since H is an invariant subgroup of g_t, the group g_t may be written as

$$g_t = H, q^*H \text{ or}$$
$$g_t = H, Hq^*$$

where for example, the elements in the left coset q^*H are $q^*p_1, q^*p_2, \ldots$, and where $q^*p_i \equiv q_i^*$. A group of the type g_t is therefore constructed from H and one element q not in H. Since all of the p_i belong to H, all the twin elements q_i^* in g_t are equivalent. That is, they all imply two individuals of a twin related to each other in exactly the same way. Therefore, the group g_t so defined expresses the symmetry

of each of the two individuals of the twin and enumerates a possible twin operation as well as all possible twin operations equivalent to this twin operation. In order to make the notation as explicit as possible, the group g_t will be written in the general form $H;q^*$.

Reticular Merohedry Twin Notation

Except for a slight modification for cubic crystals which will be discussed later, the notation employed for twinning by reticular merohedry is the same as that used for twinning by merohedry.

Construction of the Twin Groups

The problem of finding all of the possible merohedry and reticular merohedry twin groups may be broken into two parts:

1. The construction of the set of point groups $\{g_p\}$ from which a set of point groups $\{g_t\}$ may be selected where the set $\{g_t\}$ are those groups which describe all of the possible point symmetry twin relations.
2. The selection of the set $\{g_t\}$.

1. The Shubnikov space groups which are not gray may be divided into three general types: S_1, S_2, and S_3. To describe these, let T_i represent a pure translation operation of the symmetry. Let A_i represent any one of the other operations of the space group symmetry.

The three general types may then be written symbolically in terms of the types of operations they contain:

$$S_1 = A_i, T_i$$
$$S_2 = A_i, A'_j, T_i$$
$$S_3 = A_i, A'_j, T_i, T'_j$$

where the identity E may be thought of as one of the operations of the set $\{A_i\}$.

The point group operation a_i corresponding to A_i may be found by replacing the translational part, if any, of A_i, with the identity E. The point group operations corresponding to A'_j, T_i and T'_j are then a'_j, E, and E' respectively.

Consider now the Heesch point groups corresponding to groups of type S_1. These groups are the well known 32 point groups any one of which may be written as $\{a_i\}$. Therefore, any point group belonging to the set $\{g_p\}$ which could describe a twin in a crystal with space group type S_1 can contain only two kinds of operations: a_i and a^*_j where a^*_j is a possible operation which carries one individual of a twin edifice into another. This group type may be written as $\{a_i, a^*_j\}$. Groups of this type are isomorphic to the 58 black-white Heesch point groups. Groups of the type $\{a_i, a^*_i\}$ are not considered as possible twin groups since they contain the operation E^*. These are isomorphic to the 32 gray Heesch groups.

A Heesch group corresponding to a group of type S_2 contains only operations of the type a_i and a'_j and may be written symbolically as $\{a_i, a'_j\}$. Therefore any point group in the

set $\{g_p\}$ which could describe a twin in a crystal with space group type S_2 can have only operations of the type: a_i, a_j', a_k^* and $a_\ell'^*$. There are two general kinds of these groups; one contains a subgroup of index two of the type $\{a_i\}$ with the rest of the operators of the type $a_j'^*$. A group of this kind may be written as $\{a_i, a_j'^*\}$. There are 58 of these since they are isomorphic to the 58 black-white Heesch groups. The second kind of group is that which has as a subgroup of index two one of the black-white Heesch groups. This kind contains all four possible types of operations and may be written as $\{a_i, a_j', a_k^*, a_\ell'^*\}$. There are 111 such groups. These groups are constructed in the following way. Start with the Heesch group $\{a_i, a_j'\}$. Find all Heesch groups for which $\{a_i, a_j'\}$ is a subgroup of order two. In these groups place an asterisk over those elements which are not contained in the original Heesch group $\{a_i, a_j'\}$.

Finally, consider those Heesch groups corresponding to groups of type S_3. Any one of these may be written as $\{a_i, a_i'\}$. Therefore, any point group in the set $\{g_p\}$ which could describe a twin in a crystal with space group type S_3 can contain only operations of type a_i, a_i', a_j^* and $a_k'^*$; that is, groups which contain E' but not E^*. The following argument shows that the only possible groups of this type may be written as

$$a_i, a_i', a_j^*, a_j'^*.$$

1. According to the above, every conceivable group must contain operations of the type a_i and a_i'. Suppose those of type a_j^* are also in the group. Then $E'a_j^* = a_j'^*$. Since no other types of operations satisfy the group requirements, the operations $a_k'^*$ above may be written as the special type $a_j'^*$.

2. Suppose we start with only the operations a_i, a_i' and $a_j'^*$. Then $E'a_j'^* = a_j^*$ and again no other operations satisfy the group requirements.

The groups of type $\{a_i, a_i', a_j^*, a_j'^*\}$ may be constructed by introducing the element E' into the group $\{a_i, a_j^*\}$. There are therefore just 58 of the groups $\{a_i, a_i', a_j^*, a_j'^*\}$.

The following table summarizes the above*.

Shubnikov Space Group Type		Corresponding Heesch Point Group Type	Group Types in the Set $\{g_p\}$
S_1	A_i, T_i	$\{a_i\}^{32}$	$\{a_i, a_j^*\}^{58}$
S_2	$A_i A_j', T_i$	$\{a_i, a_j'\}^{58}$	$\{a_i, a_j'^*\}^{58}; \{a_i, a_j', a_k^*, a_l'^*\}^{111}$
†S_3	A_i, A_j', T_i, T_j'	$\{a_i, a_i'\}^{32}$	$\{a_i, a_j^*, a_i', a_j'^*\}^{58}$

Specific and general examples of the multiplication tables for these groups in the right-hand column above, are shown on pg. 74.

From the above, the set $\{g_p\}$ contains 285 groups. The original 90 non-gray Heesch groups are listed in Table 19 at

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*$\{\ \}^N$ denotes N groups of type $\{\ \}$.

† Included in S_3 is the group P_g1, even though it contains no elements $A_j'^3$.

Group Type and Symbol of Specific Group	Specific Example of Multiplication Table	General Multiplication Table
$\{a_i, a_j^*\}$ $2; P_y^*$	$\begin{array}{c\|cccc} & E & L_{2y} & P_y^* & C^* \\ \hline E & E & L_{2y} & P_y^* & C^* \\ L_{2y} & L_{2y} & E & C^* & P_y^* \\ P_y^* & P_y^* & C^* & E & L_{2y} \\ C^* & C^* & P_y^* & L_{2y} & E \end{array}$	$\begin{array}{c\|c} \{a_i\} & [a_j^*] \\ \hline [a_j^*] & \{a_i\} \end{array}$
$\{a_i, a_j'^*\}$ $2; P_y'^*$	$\begin{array}{c\|cccc} & E & L_{2y} & P_y'^* & C'^* \\ \hline E & E & L_{2y} & P_y'^* & C'^* \\ L_{2y} & L_{2y} & E & C'^* & P_y'^* \\ P_y'^* & P_y'^* & C'^* & E & L_{2y} \\ C'^* & C'^* & P_y'^* & L_{2y} & E \end{array}$	$\begin{array}{c\|c} \{a_i\} & [a_j'^*] \\ \hline [a_j'^*] & \{a_i\} \end{array}$
$\{a_i, a_j', a_k^*, a_\ell'^*\}$ $2'; L_{2y}^*$	$\begin{array}{c\|cccc} & E & P_y' & L_{2y}^* & C'^* \\ \hline E & E & P_y' & L_{2y}^* & C'^* \\ P_y' & P_y' & E & C'^* & L_{2y}^* \\ L_{2y}^* & L_{2y}^* & C'^* & E & P_y' \\ C'^* & C'^* & L_{2y}^* & P_y' & E \end{array}$	$\begin{array}{c\|c} \{a_i, a_j'\} & [a_k^*, a_\ell'^*] \\ \hline [a_k^*, a_\ell'^*] & \{a_i, a_j'\} \end{array}$
$\{a_i, a_j^*, a_i', a_j'^*\}$ $1'; P_y^*$	$\begin{array}{c\|cccc} & E & P_y^* & E' & P_y'^* \\ \hline E & E & P_y^* & E' & P_y'^* \\ P_y^* & P_y^* & E & P_y'^* & E' \\ E' & E' & P_y'^* & E & P_y^* \\ P_y'^* & P_y'^* & E' & P_y^* & E \end{array}$	$\begin{array}{c\|c} \{a_i, a_j^*\} & [a_i', a_j'^*] \\ \hline [a_i', a_j'^*] & \{a_i, a_j^*\} \end{array}$

the end of Section III along with the group types $\{a_i, a_j^*\}$, $\{a_i, a_j'^*\}$ and $\{a_i, a_j', a_k^*, a_l'^*\}$ derived from them.

In Table 20, the groups of type $\{a_i, a_j^*, a_i', a_j'^*\}$ are listed.

The notation used in writing the symbols for groups in the set $\{g_p\}$ (except for those in Table 24) is the following: the Heesch subgroup H of index two is written followed by a semi-colon after which is written a symbol M^* or M'^* which represents respectively either an uncolored or colored twin operation contained in the twin group.

2. The first step in the selection of the set of possible twin groups $\{g_t\}$ from the set $\{g_p\}$ may be accomplished by choosing for each Heesch group all those groups in $\{g_p\}$ for which that Heesch group is a subgroup of order two. This listing is shown in Table 21.

The merohedry twin groups corresponding to each Heesch group may be found from the above listing. They are those groups to the right of the Heesch group which belong to the same symmetry system as that particular Heesch group. The merohedry twin groups are listed in Table 22.

There are two kinds of merohedry twin groups for crystals with Heesch groups of the type $\{a_i\}$. One kind has the form $H;M^*$ where H is the uncolored Heesch group $\{a_i\}$ which represents the point symmetry of any individual of the twin edifice. These twin groups are the same as found by Curien and Le Corre. The other kind has the form $H;M'^*$ where every twin operation is a colored operation.

The merohedry twin groups for crystals with Heesch groups of the type $\{a_i, a_j'\}$ are of only one kind but have symbols of the form $H;M^*$ and $H;M'^*$ where H is the black-white Heesch group $\{a_i, a_j'\}$. The form $H;M'^*$ has been used rarely and only for the purpose of avoiding identical symbols for two different groups.

The merohedry twin groups for crystals with Heesch groups of the type $\{a_i, a_i'\}$ arise from twinning possibilities in black-white lattices. These twin groups have symbols of the form $H;M^*$ where H is the gray Heesch group $\{a_i, a_i'\}$. It is interesting to note that in this case for every possible twin operation M^* its colored companion M'^* also exists in the twin group.

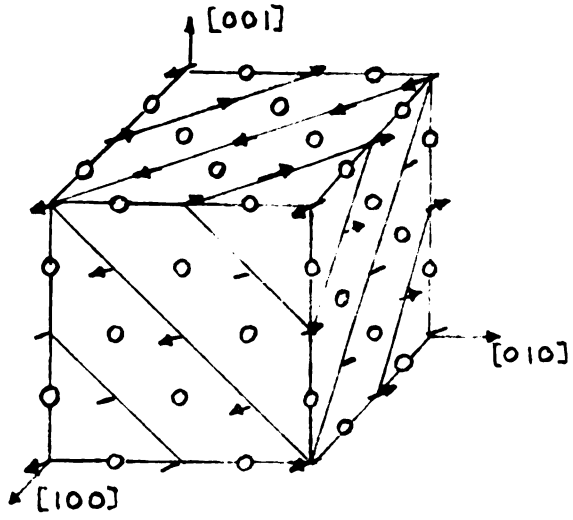
The reticular merohedry twin groups for rhombohedral crystals are listed in Table 23. The classification of these groups by the type of their Heesch subgroups of index two is the same as above for merohedry twin groups. For example, those groups of the form $H;M^*$ where H is an uncolored Heesch group are the same as found by Curien and Le Corre.

The possible reticular merohedry twin groups for cubic crystals are the same as those for rhombohedral crystals. Following Curien and Le Corre, the cubic case is distinguished from the rhombohedral case by writing in front of the rhombohedral twin group that cubic group which contains the rhombohedral Heesch group as a proper subgroup. These groups are listed in Table 24.

Twins in antiferromagnetic NiO

The only antiferromagnetic twins which seem to have been studied to date are those investigated by Roth[29] and Slack[30] in NiO. This crystal is cubic above the Néel temperature of 523°K. Below this temperature the cube contracts slightly along one of its four-body diagonals. The symmetry of the ions then becomes rhombohedral with a rhombohedral angle $\alpha = 90°4'$ for a multiple rhombohedral cell containing 4NiO. The magnetic moments associated with the Ni ions form ferromagnetic sheets which are perpendicular to the contraction axis. If the contraction axis is [111], the sheets are parallel to (111). The spin direction is then $[1\bar{1}0]$ and the spins in adjacent sheets have opposite senses. This cell is shown in Fig. 22 (Fig. 1 in Roth's paper) where the open circles represent oxygen atoms.

Fig. 22. Antiferromagnetic Structure of NiO



29. W. L. Roth, J. of Appl. Phys. 31, 2000 (1960).

30. G. A. Slack, J. of Appl. Phys. 31, 1571 (1960).

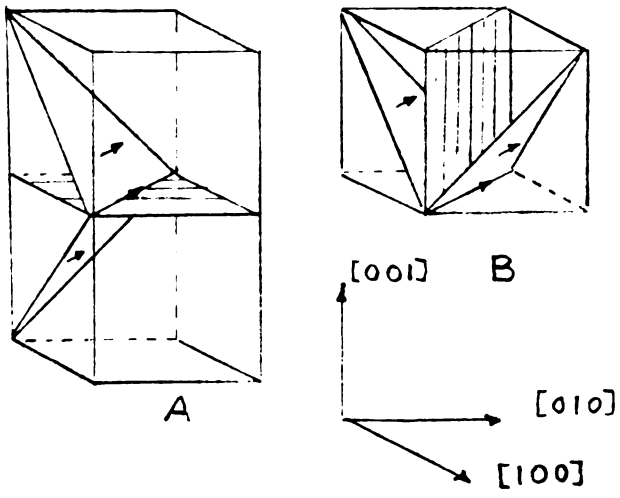
The "T domain walls" which are the observed twin planes for the antiferromagnetic twins are restricted by the conditions given on page 2002 in Roth's paper:

a. "The ferromagnetic sheets in adjoining domains intersect along a common magnetization direction and

b. the domain wall contains this direction and is parallel to a mirror plane in the original cubic crystal."

Two examples are shown in Fig. 23 (Fig. 5 in Roth's paper)

Fig. 23. T walls in NiO



In an attempt to apply the twin theory developed in this section to these NiO twins, three general possibilities must be investigated:

1. Twinning by merohedry

2. Twinning by reticular merohedry

3. Twinning by some other method

1. Twinning by Merohedry The point group symmetry of each member of the twin (in this case each domain such as that shown in Fig. 22) must first be found. This can be done in this case since the magnetic structure is known. The space symmetry of the ions is rhombohedral, however, the magnetic moments do not have the three-fold symmetry required by the rhombohedral cell. This implies a triclinic Shubnikov group symmetry. Therefore, the Heesch point group symmetry is also triclinic. Since no triclinic lattice contains a symmetry plane, the twin planes in NiO are not merohedry twin planes.

2. Twinning by Reticular Merohedry This possibility is also ruled out since this type of twinning does not take place in triclinic crystals.

3. Twinning by Some Other Method The twinning in NiO can be described by twinning by pseudo-merohedry. Possible pseudo-merohedry twin planes are planes which are parallel to planes which are almost planes of symmetry of the lattice. The planes which are almost planes of symmetry of the anti-ferromagnetic lattice of NiO are the planes of symmetry of the cubic lattice F_s. This lattice contains anti-translations along all three edges. If the rhombohedral distortion is neglected, there are only two planes compatible with the lattice F_s which are planes of symmetry of Fig. 22 and which also satisfy the requirements a and b above. One of these

is an antimirror plane parallel to (001) and the other is an antiglide plane parallel to (110). These planes are just those domain walls shown in Fig. 23.*

If the magnetic axis is changed to any one of the other observed directions shown in Table I, page 2092, of Roth's paper, there again exist just two planes similar to the two found above which may be chosen from F_s and which satisfy conditions a and b above. These planes are the domain walls listed in Table I under that particular direction of the magnetic axis.

*The point group equivalent of the glide plane will also produce the observed twin.

Table 19. The 90 non-gray Heesch Groups and the derived Group Types $\{a_i, a_j^*\}$, $\{a_i, a_j'^*\}$ and $\{a_i, a_j', a_k^*, a_l'^*\}$

Group	Elements
1	E
$\bar{1}$	E, C
$1;C^*$	E, C^*
$\bar{1}'$	E, C'
$1;C'^*$	E, C'^*
2	E, L_{2z}
$1;L_{2z}^*$	E, L_{2z}^*
2'	E, L_{2z}'
$1;L_{2z}'^*$	E, $L_{2z}'^*$
m	E, P_y
$1;P_y^*$	E, P_y^*
m'	E, P_y'
$1;P_y'^*$	E, $P_y'^*$
2/m	E, L_{2y}, P_y, C
$2;P_y^*$	E, L_{2y}, P_y^*, C^*
$m;L_{2y}^*$	E, P_y, L_{2y}^*, C^*
$\bar{1};L_{2y}^*$	E, C, L_{2y}^*, P_y^*
2/m'	E, L_{2y}, P_y', C'
$2;P_y'^*$	E, L_{2y}, $P_y'^*$, C'^*
$m';L_{2y}^*$	E, P_y', L_{2y}^*, C'^*
$\bar{1}';L_{2y}^*$	E, C', L_{2y}^*, $P_y'^*$

The symbol definitions given below are the same as those in reference 10

L_2, L_3, L_3^{-1}, L_4, L_4^{-1}, L_6, L_6^{-1} are rotations by 180, 120, -120, 90, -90, 60 and -60 degrees respectively. S_3, S_3^{-1}, S_4, S_4^{-1}, S_6, S_6^{-1} are respectively rotations by 120, -120, 90, -90, 60 and -60 degrees together with reflection in a plane at right angles to the axis of rotation. The inversion is C and P the reflection plane.

The subscripts x, y, z, xy, $\overline{xy}$, on L_i and S_i indicate the direction of the axis of rotation; the same subscripts on P indicate the direction of the normal to the plane of reflection.

The subscript $\perp$ or $\parallel$ indicates that the axis of rotation through 180° or the reflection plane is perpendicular or parallel to the main crystal axis of three-fold or higher symmetry.

$2'/m$	E, P_y, L'_{2y}, C'
$m;L'^{*}_{2y}$	$E, P_y, L'^{*}_{2y}, C'^{*}$
$2';P^{*}_{y}$	$E, L'_{2y}, P^{*}_{y}, C'^{*}$
$\bar{1}';P^{*}_{y}$	$E, C', P^{*}_{y}, L'^{*}_{2y}$
$2'/m'$	E, C, L'_{2y}, P'_{y}
$\bar{1};L'^{*}_{2y}$	$E, C, L'^{*}_{2y}, P'^{*}_{y}$
$2';C^{*}$	$E, L'_{2y}, C^{*}, P'^{*}_{y}$
$m';C^{*}$	$E, P'_{y}, C^{*}, L'^{*}_{2y}$
222	$E, L_{2x}, L_{2y}, L_{2z}$
$2;L^{*}_{2x}$	$E, L_{2z}, L^{*}_{2x}, L^{*}_{2y}$
$2'2'2$	$E, L_{2z}, L'_{2x}, L'_{2y}$
$2;L'^{*}_{2x}$	$E, L_{2z}, L'^{*}_{2x}, L'^{*}_{2y}$
$2';L^{*}_{2z}$	$E, L'_{2y}, L^{*}_{2z}, L'^{*}_{2x}$
mm	E, L_{2z}, P_x, P_y
$2;P^{*}_{x}$	$E, L_{2z}, P^{*}_{x}, P^{*}_{y}$
$m;L^{*}_{2z}$	$E, P_y, L^{*}_{2z}, P^{*}_{x}$
$m'm'$	$E, L_{2z}, P'_{x}, P'_{y}$
$2;P'^{*}_{x}$	$E, L_{2z}, P'^{*}_{x}, P'^{*}_{y}$
$m';L^{*}_{2z}$	$E, P'_{y}, L^{*}_{2z}, P'^{*}_{x}$
mm'	E, P_y, L'_{2z}, P'_{x}
$m;L'^{*}_{2z}$	$E, P_y, L'^{*}_{2z}, P'^{*}_{x}$
$2';P'^{*}_{x}$	$E, L'_{2z}, P^{*}_{y}, P'^{*}_{x}$
$m';P^{*}_{y}$	$E, P'_{x}, P^{*}_{y}, L'^{*}_{2z}$
mmm	$E, L_{2x}, L_{2y}, L_{2z}, P_x, P_y, P_z, C$
$222;P^{*}_{x}$	$E, L_{2x}, L_{2y}, L_{2z}, P^{*}_{x}, P^{*}_{y}, P^{*}_{z}, C^{*}$
$mm;L^{*}_{2x}$	$E, L_{2z}, P_x, P_y, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{z}, C^{*}$
$2/m;L^{*}_{2x}$	$E, L_{2z}, P_z, C, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{x}, P^{*}_{y}$

$m'm'm'$	$E, L_{2x}, L_{2y}, L_{2z}, P'_x, P'_y, P'_z, C'$
$222;P'^*_x$	$E, L_{2x}, L_{2y}, L_{2z}, P'^*_x, P'^*_y, P'^*_z, C'^*$
$m'm';L^*_{2x}$	$E, L_{2z}, P'_x, P'_y, L^*_{2x}, L^*_{2y}, P'^*_z, C'^*$
$2/m';L^*_{2x}$	$E, L_{2y}, P'_y, C', L^*_{2x}, L^*_{2z}, P'^*_x, P'^*_z$
mmm'	$E, L_{2z}, P_x, P_y, L'_{2x}, L'_{2y}, P'_z, C'$
$mm;L'^*_{2x}$	$E, L_{2z}, P_x, P_y, L'^*_{2x}, L'^*_{2y}, P'^*_z, C'^*$
$2/m';P^*_x$	$E, L_{2z}, P'_z, C', P^*_x, P^*_y, L'^*_{2x}, L'^*_{2y}$
$2'2'2;P^*_x$	$E, L_{2z}, L'_{2x}, L'_{2y}, P^*_x, P^*_y, P'^*_z, C'^*$
$mm';L^*_{2z}$	$E, P_x, L'_{2y}, P'_z, L^*_{2z}, P^*_y, L'^*_{2x}, C'^*$
$2'/m;L^*_{2z}$	$E, P_y, L'_{2y}, C', L^*_{2z}, P^*_x, L'^*_{2x}, P'^*_z$
$m'm'm$	$E, L_{2z}, P_z, C, L'_{2x}, L'_{2y}, P'_x, P'_y$
$2/m;L'^*_{2x}$	$E, L_{2z}, P_z, C, L'^*_{2x}, L'^*_{2y}, P'^*_x, P'^*_y$
$mm';C^*$	$E, P_z, L'_{2y}, P'_x, L^*_{2z}, C^*, L'^*_{2x}, P'^*_y$
$m'm';P^*_z$	$E, L_{2z}, P'_x, P'_y, P^*_z, C^*, L'^*_{2x}, L'^*_{2y}$
$2'2'2;P^*_z$	$E, L_{2z}, L'_{2x}, L'_{2y}, P^*_z, C^*, P'^*_x, P'^*_y$
$2'/m';L^*_{2z}$	$E, C, L'_{2y}, P'_y, L^*_{2z}, P^*_z, L'^*_{2x}, P'^*_x$
4	$E, L_{4z}, L^{-1}_{4z}, L_{2z}$
$2;L^*_{4z}$	$E, L_{2z}, L^*_{4z}, L^{-1*}_{4z}$
$4'$	$E, L_{2z}, L'_{4z}, L^{-1'}_{4z}$
$2;L'^*_{4z}$	$E, L_{2z}, L'^*_{4z}, L^{-1'*}_{4z}$
42	$E, L_{4z}, L^{-1}_{4z}, L_{2x}, L_{2y}, L_{2z}, L_{2xy}, L_{2\overline{xy}}$
$4;L^*_{2x}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, L^*_{2x}, L^*_{2y}, L^*_{2xy}, L^*_{2\overline{xy}}$
$222;L^*_{4z}$	$E, L_{2x}, L_{zy}, L_{2z}, L^*_{4z}, L^{-1*}_{4z}, L^*_{2xy}, L_{2\overline{xy}}$
$42'$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, L'_{2x}, L'_{2y}, L'_{2xy}, L'_{2\overline{xy}}$
$4;L'^*_{2x}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, L'^*_{2x}, L'^*_{2y}, L'^*_{2xy}, L'^*_{2\overline{xy}}$
$2'2'2;L^*_{4z}$	$E, L_{2z}, L'_{2x}, L'_{2y}, L^*_{4z}, L^{-1*}_{4z}, L'^*_{2xy}, L'^*_{2\overline{xy}}$

$4'2$	$E, L_{2x}, L_{2y}, L_{2z}, L'_{4z}, L^{-1}_{4z}, L'_{2xy}, L'_{2\overline{xy}}$
$222; L'^{*}_{4z}$	$E, L_{2x}, L_{2y}, L_{2z}, L'^{*}_{4z}, L^{-1}_{4z}{}'^{*}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}$
$4'; L^{*}_{2x}$	$E, L_{2x}, L'_{4z}, L^{-1}_{4z}{}', L^{*}_{2x}, L^{*}_{2y}, L'^{*}_{2xy}, L'^{*}_{2\overline{xy}}$
$4/m$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P_z, S_{4z}, S^{-1}_{4z}, C$
$4; P^{*}_{z}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P^{*}_{z}, S^{*}_{4z}, S^{-1*}_{4z}, C^{*}$
$2/m; L^{*}_{4z}$	$E, L_{2z}, P_z, C, L^{*}_{4z}, L^{-1*}_{4z}, S^{*}_{4z}, S^{-1*}_{4z}$
$\bar{4}; L^{*}_{4z}$	$E, L_{2z}, S_{4z}, S^{-1}_{4z}, L^{*}_{4z}, L^{-1*}_{4z}, P^{*}_{z}, C^{*}$
$4/m'$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'_{z}, S'_{4z}, S^{-1}_{4z}{}', C'$
$4; P'^{*}_{z}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'^{*}_{z}, S'^{*}_{4z}, S^{-1}_{4z}{}'^{*}, C'^{*}$
$\bar{4}'; L^{*}_{4z}$	$E, L_{2z}, S'_{4z}, S^{-1}_{4z}{}', L^{*}_{4z}, L^{-1*}_{4z}, P'^{*}_{z}, C'^{*}$
$2/m'; L^{*}_{4z}$	$E, L_{2z}, P'_{z}, C', L^{*}_{4z}, L^{-1*}_{4z}, S'^{*}_{4z}, S^{-1}_{4z}{}'^{*}$
$4'/m$	$E, L_{2z}, P_z, C, L'_{4z}, L^{-1}_{4z}{}', S'_{4z}, S^{-1}_{4z}{}'$
$2/m; L'^{*}_{4z}$	$E, L_{2z}, P_z, C, L'^{*}_{4z}, L^{-1}_{4z}{}'^{*}, S'^{*}_{4z}, S^{-1}_{4z}{}'^{*}$
$4'; P^{*}_{z}$	$E, L_{2z}, L'_{4z}, L^{-1}_{4z}{}'. P^{*}_{z}, C^{*}, S'^{*}_{4z}, S^{-1}_{4z}{}'^{*}$
$\bar{4}'; P^{*}_{z}$	$E, L_{2z}, S'_{4z}, S^{-1}_{4z}{}', P^{*}_{z}, C^{*}, L'^{*}_{4z}, L^{-1}_{4z}{}'^{*}$
$4'/m'$	$E, L_{2z}, S_{4z}, S^{-1}_{4z}, L'_{4z}, L^{-1}_{4z}{}', P'_{z}, C'$
$\bar{4}; L'^{*}_{4z}$	$E, L_{2z}, S_{4z}, S^{-1}_{4z}, L'^{*}_{4z}, L^{-1}_{4z}{}'^{*}, P'^{*}_{z}, C'^{*}$
$4'; S^{*}_{4z}$	$E, L_{2z}, L'_{4z}, L^{-1}_{4z}{}', S^{*}_{4z}, S^{-1*}_{4z}, P'^{*}_{z}, C'^{*}$
$2/m'; S^{*}_{4z}$	$E, L_{2z}, P'_{z}, C', S^{*}_{4z}, S^{-1*}_{4z}, L^{-1}_{4z}{}'^{*}, L'^{*}_{4z}$
$4mm$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P_x, P_y, P_{xy}, P_{\overline{xy}}$
$4; P^{*}_{x}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P^{*}_{x}, P^{*}_{y}, P^{*}_{xy}, P^{*}_{\overline{xy}}$
$mm; L^{*}_{4z}$	$E, L_{2z}, P_x, P_y, L^{*}_{4z}, L^{-1*}_{4z}, P^{*}_{xy}, P^{*}_{\overline{xy}}$
$4m'm'$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'_{x}, P'_{y}, P'_{xy}, P'_{\overline{xy}}$
$4; P'^{*}_{x}$	$E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'^{*}_{x}, P'^{*}_{y}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$
$m'm'; L^{*}_{4z}$	$E, L_{2z}, P'_{x}, P'_{y}, L^{*}_{4z}, L^{-1*}_{4z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4'mm'$ $E, L_{2z}, P_x, P_y, L'_{4z}, L^{-1'}_{4z}, P'_{xy}, P'_{\overline{xy}}$

$m'm';L'^{*}_{4z}$ $E, L_{2z}, P'_{xy}, P'_{\overline{xy}}, P^{*}_{x}, P^{*}_{y}, L'^{*}_{4z}, L^{-1'*}_{4z}$

$mm;L'^{*}_{4z}$ $E, L_{2z}, P_x, P_y, L'^{*}_{4z}, L^{-1'*}_{4z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4';P^{*}_{x}$ $E, L_{2z}, L'_{4z}, L^{-1'}_{4z}, P^{*}_{x}, P^{*}_{y}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4/mmm$ $E, L_{4z}, L^{-1}_{4z}, L_{2x}, L_{zy}, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P_x, P_y, P_z, P_{xy}, P_{\overline{xy}}, S_{4z}, S^{-1}_{4z}, C$

$42;P^{*}_{x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2x}, L_{2y}, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P^{*}_{x}, P^{*}_{y}, P^{*}_{z}, P^{*}_{xy}, P^{*}_{\overline{xy}}, S^{*}_{4z}, S^{-1*}_{4z}, C^{*}$

$4/m;L^{*}_{2x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2z}, P_z, S_{4z}, S^{-1}_{4z}, C, L^{*}_{2x}, L^{*}_{2y}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P^{*}_{x}, P^{*}_{y}, P^{*}_{xy}, P^{*}_{\overline{xy}}$

$4mm;L^{*}_{2x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2z}, P_x, P_y, P_{xy}, P_{\overline{xy}}, L^{*}_{2x}, L^{*}_{2y}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P^{*}_{z}, S^{*}_{4z}, S^{-1*}_{4z}, C^{*}$

$mmm;L^{*}_{4z}$ $E, L_{2x}, L_{2y}, L_{2z}, P_x, P_y, P_z, C, L^{*}_{4z}, L^{-1*}_{4z}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P^{*}_{xy}, P^{*}_{\overline{xy}}, S^{*}_{4z}, S^{-1*}_{4z}$

$\overline{4}2m;L^{*}_{4z}$ $E, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P_x, P_y, S_{4z}, S^{-1}_{4z}, L^{*}_{4z}, L^{-1*}_{4z}, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{z}, P^{*}_{xy}, P^{*}_{\overline{xy}}, C^{*}$

$4/m'm'm'$ $E, L_{4z}, L^{-1}_{4z}, L_{2x}, L_{2y}, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P'_{x}, P'_{y}, P'_{z}, P'_{xy}, P'_{\overline{xy}}, S'_{4z}, S^{-1'}_{4z}, C'$

$\overline{4}'2m';L^{*}_{4z}$ $E, L_{2z}, L_{2xy}, L_{2\overline{xy}}, S'_{4z}, S^{-1'}_{4z}, P'_{x}, P'_{y}, L^{*}_{4z}, L^{-1*}_{4z}, L^{*}_{2x}, L^{*}_{2y}, P'^{*}_{z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, C'^{*}$

$4m'm';L^{*}_{2x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'_{x}, P'_{y}, P'_{xy}, P'_{\overline{xy}}, L^{*}_{2x}, L^{*}_{2y}, L^{*}_{2\overline{xy}}, P'^{*}_{z}, S'^{*}_{4z}, S^{-1'*}_{4z}, C'^{*}$

$42;P'^{*}_{x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2x}, L_{2y}, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P'^{*}_{x}, P'^{*}_{y}, P'^{*}_{z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, S'^{*}_{4z}, S^{-1'*}_{4z}, C'^{*}$

$m'm'm';L^{*}_{4z}$ $E, L_{2x}, L_{2y}, L_{2z}, P'_{x}, P'_{y}, P'_{z}, C', L^{*}_{4z}, L^{-1*}_{4z}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, S'^{*}_{4z}, S^{-1'*}_{4z}$

$4/m';L^{*}_{2x}$ $E, L_{4z}, L^{-1}_{4z}, L_{2z}, P'_{z}, S'_{4z}, S^{-1'}_{4z}, C', L^{*}_{2x}, L^{*}_{2y}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P'^{*}_{x}, P'^{*}_{y}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4/m'm'm$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_z, S_{4z}, S_{4z}^{-1}, C, L_{2x}', L_{2y}', L_{2xy}', L_{2\overline{xy}}', P_x', P_y', P_{xy}', P_{\overline{xy}}'$

$4/m; L_{2x}'^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_z, S_{4z}, S_{4z}^{-1}, C, L_{2x}'^*, L_{2y}'^*, L_{2xy}'^*, L_{2\overline{xy}}'^*, P_x'^*, P_y'^*, P_{xy}'^*, P_{\overline{xy}}'^*$

$\bar{4}2m'; L_{4z}^*$ $E, S_{4z}, S_{4z}^{-1}, L_{2z}, L_{2xy}', L_{2\overline{xy}}', P_x', P_y', L_{4z}^*, L_{4z}^{-1*}, P_z^*, C^*, L_{2x}'^*, L_{2y}'^*, P_{xy}'^*, P_{\overline{xy}}'^*$

$4m'm'; P_z^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_x', P_y', P_{xy}', P_{\overline{xy}}', P_z^*, S_{4z}^*, S_{4z}^{-1*}, C^*, L_{2x}'^*, L_{2y}'^*, L_{2xy}'^*, L_{2\overline{xy}}'^*$

$42'; P_z^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, L_{2x}', L_{2y}', L_{2xy}', L_{2\overline{xy}}', P_z^*, S_{4z}^*, S_{4z}^{-1*}, C^*, P_x'^*, P_y'^*, P_{xy}'^*, P_{\overline{xy}}'^*$

$m'm'm; L_{4z}^*$ $E, L_{2z}, P_z, C, L_{2x}', L_{2y}', P_x', P_y', L_{4z}^*, L_{4z}^{-1*}, S_{4z}^*, S_{4z}^{-1*}, L_{2xy}'^*, L_{2\overline{xy}}'^*, P_{xy}'^*, P_{\overline{xy}}'^*$

$4/mmm'$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_x, P_y, P_{xy}, P_{\overline{xy}}, L_{2x}', L_{2y}', L_{2xy}', L_{2\overline{xy}}', P_z', S_{4z}', S_{4z}^{-1}', C'$

$4mm; L_{2x}'^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_x, P_y, P_{xy}, P_{\overline{xy}}, L_{2x}'^*, L_{2y}'^*, L_{2xy}'^*, L_{2\overline{xy}}'^*, P_z'^*, S_{4z}'^*, S_{4z}^{-1}'^*, C'^*$

$\bar{4}'2m; L_{4z}^*$ $E, L_{2z}, P_x, P_y, S_{4z}', S_{4z}^{-1}', L_{2xy}', L_{2\overline{xy}}', L_{4z}^*, L_{4z}^{-1*}, P_{xy}^*, P_{\overline{xy}}^*, L_{2x}'^*, L_{2y}'^*, P_z'^*, C'^*$

$4/m'; P_x^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_z', S_{4z}', S_{4z}^{-1}', C', P_x^*, P_y^*, P_{xy}^*, P_{\overline{xy}}^*, L_{2x}'^*, L_{2y}'^*, L_{2xy}'^*, L_{2\overline{xy}}'^*$

$42'; P_x^*$ $E, L_{4z}, L_{4z}^{-1}, L_{2z}, L_{2x}', L_{2y}', L_{2xy}', L_{2\overline{xy}}', P_x^*, P_y^*, P_{xy}^*, P_{\overline{xy}}^*, P_z'^*, S_{4z}'^*, S_{4z}^{-1}'^*, C'^*$

$mmm'; L_{4z}^*$ $E, L_{2z}, P_x, P_y, L_{2x}', L_{2y}', P_z', C', L_{4z}^*, L_{4z}^{-1*}, P_{xy}^*, P_{\overline{xy}}^*, L_{2xy}'^*, L_{2\overline{xy}}'^*, S_{4z}'^*, S_{4z}^{-1}'^*$

$4'/mmm$ $E, L_{2x}, L_{2y}, L_{2z}, P_x, P_y, P_z, C, L'_{4z}, L^{-1'}_{4z}, L'_{2xy}, L'_{2\overline{xy}}, P'_{xy}, P'_{\overline{xy}}, S'_{4z}, S^{-1'}_{4z}$

$mmm; L'^{*}_{4z}$ $E, L_{2x}, L_{2y}, L_{2z}, P_x, P_y, P_z, C, L'^{*}_{4z}, L^{-1'*}_{4z}, L'^{*}_{2xy}, L'^{*}_{2\overline{xy}}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, S'^{*}_{4z}, S^{-1'*}_{4z}$

$\overline{4}'2m; L^{*}_{2x}$ $E, L_{2z}, P_x, P_y, S'_{4z}, S^{-1'}_{4z}, L'_{2xy}, L'_{2\overline{xy}}, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{z}, C^{*}, L'^{*}_{4z}, L^{-1'*}_{4z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4'mm'; L^{*}_{2x}$ $E, L_{2z}, P_x, P_y, L'_{4z}, L^{-1'}_{4z}, P'_{xy}, P'_{\overline{xy}}, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{z}, C^{*}, L'^{*}_{2xy}, L'^{*}_{2\overline{xy}}, S'^{*}_{4z}, S^{-1'*}_{4z}$

$4'/m; L^{*}_{2x}$ $E, L_{2z}, P_z, C, L'_{4z}, L^{-1'}_{4z}, S'_{4z}, S^{-1'}_{4z}, L^{*}_{2x}, L^{*}_{2y}, P^{*}_{x}, P^{*}_{y}, L'^{*}_{2xy}, L'^{*}_{2\overline{xy}}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$4'2; P^{*}_{x}$ $E, L_{2x}, L_{2y}, L_{2z}, L'_{4z}, L^{-1'}_{4z}, L'_{2xy}, L'_{2\overline{xy}}, P^{*}_{x}, P^{*}_{y}, P^{*}_{z}, C^{*}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, S'^{*}_{4z}, S^{-1'*}_{4z}$

$4'/mmm'$ $E, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P_x, P_y, S_{4z}, S^{-1}_{4z}, L'_{4z}, L^{-1'}_{4z}, L'_{2x}, L'_{2y}, P'_{z}, P'_{xy}, P'_{\overline{xy}}, C'$

$4'2; S^{*}_{4z}$ $E, L_{2z}, L_{2xy}, L_{2\overline{xy}}, L'_{4z}, L^{-1'}_{4z}, L'_{2x}, L'_{2y}, P^{*}_{x}, P^{*}_{y}, S^{*}_{4z}, S^{-1*}_{4z}, P'^{*}_{z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, C'^{*}$

$\overline{4}2m; L'^{*}_{4z}$ $E, L_{2z}, L_{2xy}, L_{2\overline{xy}}, P_x, P_y, S_{4z}, S^{-1}_{4z}, L'^{*}_{4z}, L^{-1'*}_{4z}, L'^{*}_{2x}, L'^{*}_{2y}, P'^{*}_{z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}, C'^{*}$

$4'mm'; S^{*}_{4z}$ $E, L_{2z}, P_x, P_y, L'_{4z}, L^{-1'}_{4z}, P'_{xy}, P'_{\overline{xy}}, L^{*}_{2xy}, L^{*}_{2\overline{xy}}, S^{*}_{4z}, S^{-1*}_{4z}, L'^{*}_{2x}, L'^{*}_{2y}, P'^{*}_{z}, C'^{*}$

$4'/m'; P^{*}_{x}$ $E, L_{2z}, S_{4z}, S^{-1}_{4z}, L'_{4z}, L^{-1'}_{4z}, P'_{z}, C', L^{*}_{2xy}, L^{*}_{2\overline{xy}}, P^{*}_{x}, P^{*}_{y}, L'^{*}_{2x}, L'^{*}_{2y}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$mmm'; S^{*}_{4z}$ $E, L_{2z}, P_x, P_y, L'_{2x}, L'_{2y}, P'_{z}, C', L^{*}_{2xy}, L^{*}_{2\overline{xy}}, S^{*}_{4z}, S^{-1*}_{4z}, L'^{*}_{4z}, L^{-1'*}_{4z}, P'^{*}_{xy}, P'^{*}_{\overline{xy}}$

$\overline{4}$ $E, S_{4z}, S^{-1}_{4z}, L_{2z}$

$2; S^{*}_{4z}$ $E, L_{2z}, S^{*}_{4z}, S^{-1*}_{4z}$

$\bar{4}'$ E, L_{2z}, S'_{4z}, $S^{-1}{}'_{4z}$

$2;S'^{*}_{4z}$ E, L_{2z}, S'^{*}_{4z}, $S^{-1}{}'^{*}_{4z}$

$\bar{4}2m$ E, S_{4z}, S^{-1}_{4z}, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, P_x, P_y

$\bar{4};P^{*}_{x}$ E, S_{4z}, S^{-1}_{4z}, L_{2z}, L^{*}_{2xy}, $L^{*}_{2\overline{xy}}$, P^{*}_{x}, P^{*}_{y}

$222;S^{*}_{4z}$ E, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, S^{*}_{4z}, S^{-1*}_{4z}, P^{*}_{x}, P^{*}_{y}

$mm;S^{*}_{4z}$ E, L_{2z}, P_x, P_y, S^{*}_{4z}, S^{-1*}_{4z}, L^{*}_{2xy}, $L^{*}_{2\overline{xy}}$

$\bar{4}2m'$ E, S_{4z}, S^{-1}_{4z}, L_{2z}, L'_{2xy}, $L'_{2\overline{xy}}$, P'_{x}, P'_{y}

$2'2'2;S^{*}_{4z}$ E, L_{2z}, L'_{2xy}, $L'_{2\overline{xy}}$, S^{*}_{4z}, S^{-1*}_{4z}, P'^{*}_{x}, P'^{*}_{y}

$\bar{4};P'^{*}_{x}$ E, S_{4z}, S^{-1}_{4z}, L_{2z}, L'^{*}_{2xy}, $L'^{*}_{2\overline{xy}}$, P'^{*}_{x}, P'^{*}_{y}

$m'm';S^{*}_{4z}$ E, L_{2z}, P'_{x}, P'_{y}, S^{*}_{4z}, S^{-1*}_{4z}, L'^{*}_{2xy}, $L'^{*}_{2\overline{xy}}$

$\bar{4}'2m'$ E, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, S'_{4z}, $S^{-1}{}'_{4z}$, P'_{x}, P'_{y}

$222;S'^{*}_{4z}$ E, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, S'^{*}_{4z}, $S^{-1}{}'^{*}_{4z}$, P'^{*}_{x}, P'^{*}_{y}

$\bar{4}';L^{*}_{2xy}$ E, L_{2z}, S'_{4z}, $S^{-1}{}'_{4z}$, L^{*}_{2xy}, $L^{*}_{2\overline{xy}}$, P'^{*}_{x}, P'^{*}_{y}

$m'm';L^{*}_{2xy}$ E, L_{2z}, P'_{x}, P'_{y}, L^{*}_{2xy}, $L^{*}_{2\overline{xy}}$, S'^{*}_{4z}, $S^{-1}{}'^{*}_{4z}$

$\bar{4}'2m$ E, L_{2z}, P_x, P_y, S'_{4z}, $S^{-1}{}'_{4z}$, L'_{2xy}, $L'_{2\overline{xy}}$

$mm;S'^{*}_{4z}$ E, L_{2z}, P_x, P_y, S'^{*}_{4z}, $S^{-1}{}'^{*}_{4z}$, L'^{*}_{2xy}, $L'^{*}_{2\overline{xy}}$

$\bar{4}';P^{*}_{x}$ E, L_{2z}, S'_{4z}, $S^{-1}{}'_{4z}$, P^{*}_{x}, P^{*}_{y}, L'^{*}_{2xy}, $L'^{*}_{2\overline{xy}}$

$2'2'2;S'^{*}_{4z}$ E, L_{2z}, L'_{2xy}, $L'_{2\overline{xy}}$, S'^{*}_{4z}, $S^{-1}{}'^{*}_{4z}$, P^{*}_{x}, P^{*}_{y}

3 E, L_{3z}, L^{-1}_{3z}

32 E, L_{3z}, L^{-1}_{3z}, $3L_{2\perp}$

$3;L^{*}_{2\perp}$ E, L_{3z}, L^{-1}_{3z}, $3L^{*}_{2\perp}$

32' E, L_{3z}, L^{-1}_{3z}, $3L'_{2\perp}$

$3;L'^{*}_{2\perp}$ E, L_{3z}, L^{-1}_{3z}, $3L'^{*}_{2\perp}$

3m E, L_{3z}, L^{-1}_{3z}, $3P_{\parallel}$

$3;P^{*}_{\parallel}$ E, L_{3z}, L^{-1}_{3z}, $3P^{*}_{\parallel}$

3m' E, L_{3z}, L^{-1}_{3z}, $3P'_{\parallel}$

$3;P'^{*}_{\parallel}$ E, L_{3z}, L^{-1}_{3z}, $3P'^{*}_{\parallel}$

$\bar{3}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C$

$3;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}^{*}, S_{6z}^{-1*}, C^{*}$

$\bar{3}'$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}', S_{6z}^{-1'}, C'$

$3;S_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}'^{*}, S_{6z}^{-1'*}, C'^{*}$

$\bar{3}m$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, 3P_{\parallel}, 3L_{2\perp}, C$

$32;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}^{*}, S_{6z}^{-1*}, 3P_{\parallel}^{*}, C^{*}$

$3m;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{6z}^{*}, S_{6z}^{-1*}, 3L_{2\perp}^{*}, C^{*}$

$\bar{3};P_{\parallel}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, 3P_{\parallel}^{*}, 3L_{2\perp}^{*}$

$\bar{3}'m'$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}', S_{6z}^{-1'}, 3P_{\parallel}', C'$

$32;S_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}'^{*}, S_{6z}^{-1'*}, 3P_{\parallel}'^{*}, C'^{*}$

$3m';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}', 3L_{2\perp}^{*}, S_{6z}'^{*}, S_{6z}^{-1'*}, C'^{*}$

$\bar{3}';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}', S_{6z}^{-1'}, C', 3L_{2\perp}^{*}, 3P_{\parallel}'^{*}$

$\bar{3}'m$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{6z}', S_{6z}^{-1'}, 3L_{2\perp}', C'$

$3m;S_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{6z}'^{*}, S_{6z}^{-1'*}, 3L_{2\perp}'^{*}, C'^{*}$

$32';P_{\parallel}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}', 3P_{\parallel}^{*}, S_{6z}'^{*}, S_{6z}^{-1'*}, C'^{*}$

$\bar{3}';P_{\parallel}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}', S_{6z}^{-1'}, C', 3P_{\parallel}^{*}, 3L_{2\perp}'^{*}$

$\bar{3}m'$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, 3P_{\parallel}', 3L_{2\perp}'$

$\bar{3};P_{\parallel}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, 3P_{\parallel}'^{*}, 3L_{2\perp}'^{*}$

$32';S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}', S_{6z}^{*}, S_{6z}^{-1*}, C^{*}, 3P_{\parallel}'^{*}$

$3m';S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}', S_{6z}^{*}, S_{6z}^{-1*}, C^{*}, 3L_{2\perp}'^{*}$

$\bar{6}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_{z}$

$3;S_{3z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}^{*}, S_{3z}^{-1*}, P_{z}^{*}$

$\bar{6}'$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}', S_{3z}^{-1'}, P_{z}'$

$3;S_{3z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}'^{*}, S_{3z}^{-1'*}, P_{z}'^{*}$

$\bar{6}m2$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, $3L_{2\perp}$, $3P_{\parallel}$, P_z

$\bar{6};L_{2\perp}^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, $3L_{2\perp}^{*}$, $3P_{\parallel}^{*}$

$3m;S_{3z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, S_{3z}^{*}, S_{3z}^{-1*}, $3L_{2\perp}^{*}$, P_z^{*}

$32;S_{3z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, S_{3z}^{*}, S_{3z}^{-1*}, $3P_{\parallel}^{*}$, P_z^{*}

$\bar{6}m'2'$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, $3L_{2\perp}'$, $3P_{\parallel}'$

$\bar{6};L_{2\perp}'^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, $3L_{2\perp}'^{*}$, $3P_{\parallel}'^{*}$

$32';S_{3z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}'$, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, $3P_{\parallel}'^{*}$

$3m';S_{3z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}'$, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, $3L_{2\perp}'^{*}$

$\bar{6}'m2'$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, S_{3z}', S_{3z}^{-1}', $3L_{2\perp}'$, P_z'

$3m;S_{3z}'^{*}$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, $S_{3z}'^{*}$, $S_{3z}^{-1}'^{*}$, $3L_{2\perp}'^{*}$, $P_z'^{*}$

$32';S_{3z}'^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}'$, $3P_{\parallel}^{*}$, $S_{3z}'^{*}$, $S_{3z}^{-1}'^{*}$, $P_z'^{*}$

$\bar{6}';P_{\parallel}^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{3z}', S_{3z}^{-1}', P_z', $3P_{\parallel}^{*}$, $3L_{2\perp}'^{*}$

$\bar{6}'m'2$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, S'_{3z}, S_{3z}^{-1}', $3P_{\parallel}'$, P_z'

$32;S_{3z}'^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, $S_{3z}'^{*}$, $S_{3z}^{-1}'^{*}$, $3P_{\parallel}'^{*}$, $P_z'^{*}$

$3m';S_{3z}'^{*}$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}'$, $3L_{2\perp}^{*}$, $S_{3z}'^{*}$, $S_{3z}^{-1}'^{*}$, $P_z'^{*}$

$\bar{6}';L_{2\perp}^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{3z}', S_{3z}^{-1}', P_z', $3L_{2\perp}^{*}$, $3P_{\parallel}'^{*}$

6 E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}

$3;L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}

6' E, L_{3z}, L_{3z}^{-1}, L_{6z}', L_{6z}^{-1}', L_{2z}'

$3;L_{6z}'^{*}$ E, L_{3z}, L_{3z}^{-1}, $L_{6z}'^{*}$, $L_{6z}^{-1}'^{*}$, $L_{2z}'^{*}$

62 E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, $6L_{2\perp}$

$6;L_{2\perp}^{*}$ E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, $6L_{2\perp}^{*}$

$32;L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, $3L_{2\perp}^{*}$

62' E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, $6L_{2\perp}'$

$6;L_{2\perp}'^{*}$ E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, $6L_{2\perp}'^{*}$

$32';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}'$, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, $3L_{2\perp}'^{*}$

$6'2$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, L_{6z}', L_{6z}^{-1\prime}, L_{2z}', 3L_{2\perp}'$

$32;L_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, L_{6z}'^{*}, L_{6z}^{-1\prime *}, L_{2z}'^{*}, 3L_{2\perp}'^{*}$

$32';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}', 3L_{2\perp}^{*}, L_{6z}'^{*}, L_{6z}^{-1\prime *}, L_{2z}'^{*}$

$6';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}', L_{6z}^{-1\prime}, L_{2z}', 3L_{2\perp}^{*}, 3L_{2\perp}'^{*}$

$6/m$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, C$

$\bar{6};L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{6z}^{*}, S_{6z}^{-1*}, C^{*}$

$6;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{2z}, L_{6z}, L_{6z}^{-1}, S_{6z}^{*}, S_{6z}^{-1*}, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, C^{*}$

$\bar{3};L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}$

$6'/m$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, L_{6z}', L_{6z}^{-1\prime}, L_{2z}', S_{6z}', S_{6z}^{-1\prime}, C'$

$6;L_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, L_{6z}'^{*}, L_{6z}^{-1\prime *}, L_{2z}'^{*}, S_{6z}'^{*}, S_{6z}^{-1\prime *}, C'^{*}$

$\bar{3}';S_{3z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}', S_{6z}^{-1\prime}, C', S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, L_{6z}'^{*}, L_{6z}^{-1\prime *}, L_{2z}'^{*}$

$6';S_{3z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}', L_{6z}^{-1\prime}, L_{2z}', S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, S_{6z}'^{*}, S_{6z}^{-1\prime *}, C'^{*}$

$6/m'$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, S_{6z}', S_{6z}^{-1\prime}, S_{3z}', S_{3z}^{-1\prime}, P_z', C'$

$6;S_{6z}'^{*}$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, S_{6z}'^{*}, S_{6z}^{-1\prime *}, S_{3z}'^{*}, S_{3z}^{-1\prime *}, P_z'^{*}, C'^{*}$

$\bar{3}';L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}', S_{6z}^{-1\prime}, C', L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{3z}'^{*}, S_{3z}^{-1\prime *}, P_z'^{*}$

$\bar{6}';L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}', S_{3z}^{-1\prime}, P_z', L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{6z}'^{*}, S_{6z}^{-1\prime *}, C'^{*}$

$6'/m'$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, L_{6z}', L_{6z}^{-1}', L_{2z}', S_{3z}', S_{3z}^{-1}', P_z'$

$\bar{3};L_{6z}'^*$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, L_{6z}'^*, L_{6z}^{-1}'^*, L_{2z}'^*, S_{3z}'^*, S_{3z}^{-1}'^*, P_z'^*$

$\bar{6}';S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}', S_{3z}^{-1}', P_z', S_{6z}^*, S_{6z}^{-1*}, C^*, L_{6z}'^*, L_{6z}^{-1}'^*, L_{2z}'^*$

$6';S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}', L_{6z}^{-1}', L_{2z}', S_{6z}^*, S_{6z}^{-1*}, C^*, S_{3z}'^*, S_{3z}^{-1}'^*, P_z'^*$

$6mm$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, 6P_{\parallel}$

$6;P_{\parallel}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}^*$

$3m;L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, 3P_{\parallel}^*$

$6m'm'$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}'$

$6;P_{\parallel}'^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}'^*$

$3m';L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}', L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, 3P'^*$

$6'm'm$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, L_{6z}', L_{6z}^{-1}', L_{2z}', 3P_{\parallel}'$

$3m;L_{6z}'^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, L_{6z}'^*, L_{6z}^{-1}'^*, L_{2z}'^*, 3P_{\parallel}'^*$

$3m';P_{\parallel}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}', 3P_{\parallel}^*, L_{6z}'^*, L_{6z}^{-1}'^*, L_{2z}'^*$

$6';P_{\parallel}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}', L_{6z}^{-1}', L_{2z}', 3P_{\parallel}^*, 3P_{\parallel}'^*$

$6/mm$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, 6L_{2\perp}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, 6P_{\parallel}, P_z, C$

$\bar{6}m2;L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{3z}, S_{3z}^{-1}, 3P_{\parallel}, P_z, L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, 3L_{2\perp}^*, S_{6z}^*, S_{6z}^{-1*}, 3P_{\parallel}^*, C^*$

$6/m;L_{2\perp}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, C, 6L_{2\perp}^*, 6P_{\parallel}^*$

$\bar{3}m;L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}, S_{6z}^{-1}, 3P_{\parallel}, C, L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, 3L_{2\perp}^*, S_{3z}^*, S_{3z}^{-1*}, 3P_{\parallel}^*, P_z^*$

$62;S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6L_{2\perp}, S_{6z}^*, S_{6z}^{-1*}, S_{3z}^*, S_{3z}^{-1*}, 6P_{\parallel}^*, P_z^*, C^*$

$6mm;S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}, 6L_{2\perp}^*, S_{6z}^*, S_{6z}^{-1*}, S_{3z}^*, S_{3z}^{-1*}, P_z^*, C^*$

$6'/mm$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{3z}, S_{3z}^{-1}, 3P_{\parallel}, P_z, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3L_{2\perp}', S_{6z}', S_{6z}^{-1'}, 3P_{\parallel}', C'$

$\bar{6}m2;L_{6z}'^*$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{3z}, S_{3z}^{-1}, 3P_{\parallel}, P_z, L_{6z}'^*, L_{6z}^{-1'*}, L_{2z}'^*, 3L_{2\perp}'^*, S_{6z}'^*, S_{6z}^{-1'*}, 3P_{\parallel}'^*, C'^*$

$\bar{3}'m';S_{3z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}', S_{6z}^{-1'}, 3P_{\parallel}', C', S_{3z}^*, S_{3z}^{-1*}, 3P_{\parallel}^*, P_z^*, L_{6z}'^*, L_{6z}^{-1'*}, L_{2z}'^*, 3L_{2\perp}'^*$

$\bar{3}'m;S_{3z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{6z}', S_{6z}^{-1'}, 3L_{2\perp}', C', 3L_{2\perp}^*, S_{3z}^*, S_{3z}^{-1*}, P_z^*, L_{6z}'^*, L_{6z}^{-1'*}, L_{2z}'^*, 3P_{\parallel}'^*$

$\bar{6}m'2';L_{2\perp}^*$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, 3L_{2\perp}', 3P_{\parallel}', 3L_{2\perp}^*, 3P_{\parallel}^*, L_{6z}'^*, L_{6z}^{-1'*}, L_{2z}'^*, S_{6z}'^*, S_{6z}^{-1'*}, C'^*$

$6'2;S_{3z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3L_{2\perp}', S_{3z}^*, S_{3z}^{-1*}, P_z^*, S_{6z}'^*, S_{6z}^{-1'*}, 3P_{\parallel}'^*, 3P_{\parallel}^*, C'^*$

$6'/m;L_{2\perp}^*$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, L_{6z}', L_{6z}^{-1'}, L_{2z}', S_{6z}', S_{6z}^{-1'}, C', 3L_{2\perp}^*, 3P_{\parallel}^*, 3L_{2\perp}'^*, 3P_{\parallel}'^*$

$6'm'm;S_{3z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3P_{\parallel}', 3L_{2\perp}^*, S_{3z}^*, S_{3z}^{-1*}, P_z^*, 3L_{2\perp}'^*, S_{6z}'^*, S_{6z}^{-1'*}, C'^*$

$6/mm'$ $E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, C, 6L_{2\perp}', 6P_{\parallel}'$

$6/m;L_{2\perp}'^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, C, 6L_{2\perp}'^*, 6P_{\parallel}'^*$

$\bar{3}m';L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, 3P_{\parallel}', 3L_{2\perp}', L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, S_{3z}^*, S_{3z}^{-1*}, P_z^*, 3L_{2\perp}'^*, 3P_{\parallel}'^*$

$\bar{6}m'2';L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, 3L_{2\perp}', 3P_{\parallel}', L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, S_{6z}^*, S_{6z}^{-1*}, C^*, 3L_{2\perp}'^*, 3P_{\parallel}'^*$

$6m'm';S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}', S_{6z}^*, S_{6z}^{-1*}, S_{3z}^*, S_{3z}^{-1*}, P_z^*, C^*, 6L_{2\perp}'^*$

$62';S_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6L_{2\perp}', S_{6z}^*, S_{6z}^{-1*}, S_{3z}^*, S_{3z}^{-1*}, P_z^*, C^*, 6P_{\parallel}'^*$

$6'/m'm$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}, S_{6z}^{1}, 3P_{\parallel}, C, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3L_{2\perp}', S_{3z}', S_{3z}^{-1'}, 3P_{\parallel}', P_z'$

$\bar{3}m;L_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}, S_{6z}^{1}, 3P_{\parallel}, C, L_{6z}'^{*}, L_{6z}^{-1'*}, L_{2z}'^{*}, 3L_{2\perp}'^{*}, S_{3z}'^{*}, S_{3z}^{-1'*}, 3P_{\parallel}'^{*}, P_z'^{*}$

$\bar{3}m';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, 3P_{\parallel}', 3L_{2\perp}', 3L_{2\perp}^{*}, 3P_{\parallel}^{*}, L_{6z}'^{*}, L_{6z}^{-1'*}, L_{2z}'^{*}, S_{3z}'^{*}, S_{3z}^{-1'*}, P_z'^{*}$

$\bar{6}'m2';S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{3z}', S_{3z}^{-1'}, 3L_{2\perp}', P_z', 3L_{2\perp}^{*}, S_{6z}^{*}, S_{6z}^{-1*}, C^{*}, L_{6z}^{-1'*}, L_{6z}'^{*}, L_{2z}'^{*}, 3P_{\parallel}'^{*}$

$\bar{6}'m'2;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{3z}', S_{3z}^{-1'}, 3P_{\parallel}', P_z', S_{6z}^{*}, S_{6z}^{-1*}, 3P_{\parallel}^{*}, C^{*}, L_{6z}'^{*}, L_{6z}^{-1'*}, L_{2z}'^{*}, 3L_{2\perp}'^{*}$

$6'2;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3L_{2\perp}', S_{6z}^{*}, S_{6z}^{-1*}, 3P_{\parallel}^{*}, C^{*}, S_{3z}'^{*}, S_{3z}^{-1'*}, 3P_{\parallel}'^{*}, P_z'^{*}$

$6'/m';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, L_{6z}', L_{6z}^{-1'}, L_{2z}', S_{3z}', S_{3z}^{-1'}, P_z', 3L_{2\perp}^{*}, 3P_{\parallel}^{*}, 3L_{2\perp}'^{*}, 3P_{\parallel}'^{*}$

$6'm'm;S_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, L_{6z}', L_{6z}^{-1'}, L_{2z}', 3P_{\parallel}', 3L_{2\perp}^{*}, S_{6z}^{*}, S_{6z}^{-1*}, C^{*}, 3L_{2\perp}'^{*}, S_{3z}'^{*}, S_{3z}^{-1'*}, P_z'^{*}$

$6/m'm'$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6L_{2\perp}, S_{6z}', S_{6z}^{1'}, S_{3z}', S_{3z}^{-1'}, 6P_{\parallel}', P_z', C'$

$62;S_{6z}'^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6L_{2\perp}, S_{6z}'^{*}, S_{6z}^{-1'*}, S_{3z}'^{*}, S_{3z}^{-1'*}, 6P_{\parallel}'^{*}, P_z'^{*}, C'^{*}$

$\bar{3}'m';L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{6z}', S_{6z}^{-1'}, 3P_{\parallel}', C', L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, 3L_{2\perp}^{*}, S_{3z}'^{*}, S_{3z}^{-1'*}, 3P_{\parallel}'^{*}, P_z'^{*}$

$\bar{6}'m'2;L_{6z}^{*}$ $E, L_{3z}, L_{3z}^{-1}, 3L_{2\perp}, S_{3z}', S_{3z}^{-1'}, 3P_{\parallel}', P_z', L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, 3L_{2\perp}^{*}, S_{6z}'^{*}, S_{6z}^{1'*}, 3P_{\parallel}'^{*}, C'^{*}$

$6/m';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, S_{6z}', S_{6z}^{1'}, S_{3z}', S_{3z}^{-1'}, P_z', C', 6L_{2\perp}^{*}, 6P_{\parallel}'^{*}$

$6m'm';L_{2\perp}^{*}$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}', 6L_{2\perp}^{*}, S_{6z}'^{*}, S_{6z}^{1'*}, S_{3z}'^{*}, S_{3z}^{-1'*}, P_z'^{*}, C'^{*}$

$6/m'm$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}, 6L_{2\perp}', S_{6z}', S_{6z}^{-1'}, S_{3z}', S_{3z}^{-1'}, P_z', C'$

$6mm; L_{2\perp}'^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6P_{\parallel}, 6L_{2\perp}'^*, S_{6z}'^*, S_{6z}^{-1'*}, S_{3z}'^*, S_{3z}^{-1'*}, P_z'^*, C'^*$

$\bar{3}'m; L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{6z}', S_{6z}^{-1'}, 3L_{2\perp}', C', L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, 3P_{\parallel}^*, 3L_{2\perp}'^*, S_{3z}'^*, S_{3z}^{-1'*}, P_z'^*$

$\bar{6}'m2'; L_{6z}^*$ $E, L_{3z}, L_{3z}^{-1}, 3P_{\parallel}, S_{3z}', S_{3z}^{-1'}, 3L_{2\perp}', P_z', L_{6z}^*, L_{6z}^{-1*} L_{2z}^*, 3P_{\parallel}^*, 3L_{2\perp}'^*, S_{6z}'^*, S_{6z}^{-1'*}, C'^*$

$62'; P_{\parallel}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, 6L_{2\perp}', 6P_{\parallel}^*, S_{6z}'^*, S_{6z}^{-1'*}, S_{3z}'^*, S_{3z}^{-1'*}, P_z'^*, C'^*$

$6/m'; P_{\parallel}^*$ $E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, S_{6z}', S_{6z}^{-1'}, S_{3z}', S_{3z}^{-1'}, P_z', C', 6P_{\parallel}^*, 6L_{2\perp}'^*$

23 $E, 3L_2, 4L_3, 4L_3^{-1}$

$m3$ $E, 3L_2, 4L_3, 4L_3^{-1}, 4S_6, 4S_6^{-1}, 3P, C$

$23; S_6^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 4S_6^*, 4S_6^{-1*}, 3P^*, C^*$

$m'3$ $E, 3L_2, 4L_3, 4L_3^{-1}, 4S_6', 4S_6^{-1'}, 3P', C'$

$23; S_6'^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 4S_6'^*, 4S_6^{-1'*}, 3P'^*, C'^*$

$\bar{4}3m$ $E, 3L_2, 4L_3, 4L_3^{-1}, 6P, 3S_4, 3S_4^{-1}$

$23; P^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 6P^*, 3S_4^*, 3S_4^{-1*}$

$\bar{4}3m'$ $E, 3L_2, 4L_3, 4L_3^{-1}, 6P', 3S_4', 3S_4^{-1'}$

$23; P'^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 6P'^*, 3S_4'^*, 3S_4^{-1'*}$

43 $E, 3L_2, 4L_3, 4L_3^{-1}, 3L_4, 3L_4^{-1}, 6L_2$

$23; L_4^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 3L_4^*, 3L_4^{-1*}, 6L_2^*$

$4'3$ $E, 3L_2, 4L_3, 4L_3^{-1}, 3L_4', 3L_4^{-1'}, 6L_2'$

$23; L_4'^*$ $E, 3L_2, 4L_3, 4L_3^{-1}, 3L_4'^*, 3L_4^{-1'*}, 6L_2'^*$

$m3m$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4,\ 3L_4^{-1},\ 6L_2,\ 3S_4,\ 3S_4^{-1},\ 4S_6,\ 4S_6^{-1},\ 6P,\ 3P,\ C$
$43;S_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4,\ 3L_4^{-1},\ 6L_2,\ 3S_4^*,\ 3S_4^{-1*},\ 4S_6^*,\ 4S_6^{-1*},\ 6P^*,\ 3P^*,\ C^*$
$\bar{4}3m;L_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3S_4,\ 3S_4^{-1},\ 6P,\ 3L_4^*,\ 3L_4^{-1*},\ 6L_2^*,\ 4S_6^*,\ 4S_6^{-1*},\ 3P^*,\ C^*$
$m3;L_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 4S_6,\ 4S_6^{-1},\ 3P,\ C,\ 3L_4^*,\ 3L_4^{-1*},\ 6L_2^*,\ 3S_4^*,\ 3S_4^{-1*},\ 6P^*$
$m'3m'$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4,\ 3L_4^{-1},\ 6L_2,\ 3S_4',\ 3S_4^{-1'},\ 4S_6',\ 4S_6^{-1'},\ 6P',\ 3P',\ C'$
$43;S_4'^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4,\ 3L_4^{-1},\ 6L_2,\ 3S_4'^*,\ 3S_4^{-1'*},\ 4S_6'^*,\ 4S_6^{-1'*},\ 6P'^*,\ 3P'^*,\ C'^*$
$m'3;L_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 4S_6',\ 4S_6^{-1'},\ 3P',\ C',\ 3L_4^*,\ 3L_4^{-1*},\ 6L_2^*,\ 3S_4'^*,\ 3S_4^{-1'*},\ 6P'^*$
$\bar{4}3m';L_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 6P',\ 3S_4',\ 3S_4^{-1'},\ 3L_4^*,\ 3L_4^{-1*},\ 6L_2^*,\ 4S_6'^*,\ 4S_6^{-1'*},\ 3P'^*,\ C'^*$
$m3m'$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3S_4,\ 3S_4^{-1},\ 6P,\ 3L_4',\ 3L_4^{-1'},\ 6L_2',\ 4S_6',\ 4S_6^{-1'},\ 3P',\ C'$
$\bar{4}3m;L_4'^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3S_4,\ 3S_4^{-1},\ 6P,\ 3L_4'^*,\ 3L_4^{-1'*},\ 6L_2'^*,\ 4S_6'^*,\ 4S_6^{-1'*},\ 3P'^*,\ C'^*$
$m'3;S_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 4S_6',\ 4S_6^{-1'},\ 3P',\ C',\ 3S_4^*,\ 3S_4^{-1*},\ 6P^*,\ 3L_4'^*,\ 3L_4^{-1'*},\ 6L_2'^*$
$4'3;S_4^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4',\ 3L_4^{-1'},\ 6L_2',\ 3S_4^*,\ 3S_4^{-1*},\ 6P^*,\ 4S_6'^*,\ 4S_6^{-1'*},\ 3P'^*,\ C'^*$

$m'3m'$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 4S_6,\ 4S_6^{-1},\ 3P,\ C,\ 3L_4',\ 3L_4^{-1'},$ $6L_2',\ 3S_4',\ 3S_4^{-1'},\ 6P'$
$m3;L_4'^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 4S_6,\ 4S_6^{-1},\ 3P,\ C,\ 3L_4'^*,$ $3L_4^{-1'*},\ 6L_2'^*,\ 3S_4'^*,\ 3S_4^{-1'*},\ 6P'^*$
$\bar{4}3m';S_6^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 6P',\ 3S_4',\ 3S_4^{-1'},\ 4S_6^*,\ 4S_6^{-1*},$ $3P^*,\ C^*,\ 3L_4'^*,\ 3L_4^{-1'*},\ 6L_2'^*$
$4'3;S_6^*$	$E,\ 3L_2,\ 4L_3,\ 4L_3^{-1},\ 3L_4',\ 3L_4^{-1'},\ 6L_2',\ 4S_6^*,\ 4S_6^{-1*},$ $3P^*,\ C^*,\ 3S_4'^*,\ 3S_4^{-1'*},\ 6P'^*$

Table 20* Groups of Type $\{a_i, a_j^*, a_i', a_j'^*\}$

Group	Elements
$1';C^*$	E, C^*, & '
$1';L^*_{2z}$	E, L^*_{2z}, & '
$1';P^*_y$	E, P^*_y, & '
$21';P^*_y$	E, L_{2y}, P^*_y, C^*, & '
$ml';L^*_{2y}$	E, P_y, L^*_{2y}, C^*, & '
$\bar{1}1';L^*_{2y}$	E, C, L^*_{2y}, P^*_y, & '
$21';L^*_{2x}$	E, L_{2z}, L^*_{2x}, L^*_{2y}, & '
$21';P^*_x$	E, L_{2z}, P^*_x, P^*_y, & '
$ml';L^*_{2z}$	E, P_y, L^*_{2z}, P^*_x, & '
$2221';P^*_x$	E, L_{2x}, L_{2y}, L_{2z}, P^*_x, P^*_y, P^*_z, C^*, & '
$mml';L^*_{2x}$	E, L_{2z}, P_x, P_y, L^*_{2x}, L^*_{2y}, P^*_z, C^*, & '
$2/ml';L^*_{2x}$	E, L_{2z}, P_z, C, L^*_{2x}, L^*_{2y}, P^*_x, P^*_y, & '
$21';L^*_{4z}$	E, L_{2z}, L^*_{4z}, L^{-1*}_{4z}, & '
$41';L^*_{2x}$	E, L_{4z}, L^{-1}_{4z}, L_{2z}, L^*_{2x}, L^*_{2y}, L^*_{2xy}, $L^*_{2\overline{xy}}$, & '
$2221';L^*_{4z}$	E, L_{2x}, L_{2y}, L_{2z}, L^*_{4z}, L^{-1*}_{4z}, L^*_{2xy}, $L^*_{2\overline{xy}}$, & '
$41';S^*_{4z}$	E, L_{4z}, L^{-1}_{4z}, L_{2z}, P^*_z, S^*_{4z}, S^{-1*}_{4z}, C^*, & '
$2/ml';L^*_{4z}$	E, L_{2z}, P_z, C, L^*_{4z}, L^{-1*}_{4z}, S^*_{4z}, S^{-1*}_{4z}, & '
$\bar{4}1';L^*_{4z}$	E, L_{2z}, S_{4z}, S^{-1}_{4z}, L^*_{4z}, L^{-1*}_{4z}, P^*_z, C^*, & '
$41';P^*_x$	E, L_{4z}, L^{-1}_{4z}, L_{2z}, P^*_x, P^*_y, P^*_{xy}, $P^*_{\overline{xy}}$, & '
$mml';L^*_{4z}$	E, L_{2z}, P_x, P_y, L^*_{4z}, L^{-1*}_{4z}, P^*_{xy}, $P^*_{\overline{xy}}$, & '

*Unlike Table 19, all the elements in Table 20 are not written explicitly for each group. Instead, only half the elements in each group are explicitly written. The remaining half are collectively indicated by the symbols & '. To write these elements explicitly, write the elements to the left of & and then prime each of them. For example, the four elements of the first group $(1';C^*)$ are E, C^*, E', $C^{*\prime}$.

$421';P_x^*$ E, L_{4z}, L_{4z}^{-1}, L_{2x}, L_{2y}, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, P_x^*, P_y^*, P_z^*, P_{xy}^*, $P_{\overline{xy}}^*$, S_{4z}^*, S_{4z}^{-1*}, C^*, & '

$4/ml';L_{2x}^*$ E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_z, S_{4z}, S_{4z}^{-1}, C, L_{2x}^*, L_{2y}^*, L_{2xy}^*, $L_{2\overline{xy}}^*$, P_x^*, P_y^*, P_{xy}^*, $P_{\overline{xy}}^*$, & '

$4mml';L_{2x}^*$ E, L_{4z}, L_{4z}^{-1}, L_{2z}, P_x, P_y, P_{xy}, $P_{\overline{xy}}$, L_{2x}^*, L_{2y}^*, L_{2xy}^*, $L_{2\overline{xy}}^*$, P_z^*, S_{4z}^*, S_{4z}^{-1*}, C^*, & '

$mmml';L_{4z}^*$ E, L_{2x}, L_{2y}, L_{2z}, P_x, P_y, P_z, C, L_{4z}^*, L_{4z}^{-1*}, L_{2xy}^*, $L_{2\overline{xy}}^*$, P_{xy}^*, $P_{\overline{xy}}^*$, S_{4z}^*, S_{4z}^{-1*}, & '

$\bar{4}2ml';L_{4z}^*$ E, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, P_x, P_y, S_{4z}, S_{4z}^{-1}, L_{4z}^*, L_{4z}^{-1*}, L_{2x}^*, L_{2y}^*, P_z^*, P_{xy}^*, $P_{\overline{xy}}^*$, C^*, & '

$21';S_{4z}^*$ E, L_{2z}, S_{4z}^*, S_{4z}^{-1*}, & '

$\bar{4}1';L_{2xy}^*$ E, S_{4z}, S_{4z}^{-1}, L_{2z}, L_{2xy}^*, $L_{2\overline{xy}}^*$, P_x^*, P_y^*, & '

$2221';S_{4z}^*$ E, L_{2z}, L_{2xy}, $L_{2\overline{xy}}$, S_{4z}^*, S_{4z}^{-1*}, P_x^*, P_y^*, & '

$mml';S_{4z}^*$ E, L_{2z}, P_x, P_y, S_{4z}^*, S_{4z}^{-1*}, L_{2xy}^*, $L_{2\overline{xy}}^*$, & '

$31';L_{2\perp}^*$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}^*$, & '

$31';P_{\parallel}^*$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}^*$, & '

$31';S_{6z}^*$ E, L_{3z}, L_{3z}^{-1}, S_{6z}^*, S_{6z}^{-1*}, C^*, & '

$321';S_{6z}^*$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, S_{6z}^*, S_{6z}^{-1*}, $3P_{\parallel}^*$, C^*, & '

$3ml';S_{6z}^*$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, S_{6z}^*, S_{6z}^{-1*}, $3L_{2\perp}^*$, C^*, & '

$\bar{3}1';L_{2\perp}^*$ E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, $3P_{\parallel}^*$, $3L_{2\perp}^*$, & '

$31';S_{3z}^*$ E, L_{3z}, L_{3z}^{-1}, S_{3z}^*, S_{3z}^{-1*}, P_z^*, & '

$\bar{6}1';L_{2\perp}^*$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, $3L_{2\perp}^*$, $3P_{\parallel}^*$, & '

$3ml';S_{3z}^*$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, S_{3z}^*, S_{3z}^{-1*}, $3L_{2\perp}^*$, P_z^*, & '

$321';S_{3z}^*$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, S_{3z}^*, S_{3z}^{-1*}, $3P_{\parallel}^*$, P_z^*, & '

$31';L_{6z}^*$ E, L_{3z}, L_{3z}^{-1}, L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, & '

$61';L_{2\perp}^*$ E, L_{6z}, L_{6z}^{-1}, L_{3z}, L_{3z}^{-1}, L_{2z}, $6L_{2\perp}^*$, & '

$321';L_{6z}^*$ E, L_{3z}, L_{3z}^{-1}, $3L_{2\perp}$, L_{6z}^*, L_{6z}^{-1*}, L_{2z}^*, $3L_{2\perp}^*$, & '

$\bar{6}1';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{6z}^{*}, S_{6z}^{-1*}, C^{*}, & '

$61';S_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{2z}, L_{6z}, L_{6z}^{-1}, S_{6z}^{*}, S_{6z}^{-1*}, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, C^{*}, & '

$\bar{3}1';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, S_{6z}, S_{6z}^{-1}, C, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, & '

$61';P_{\parallel}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, $6P_{\parallel}^{*}$, & '

$3m1';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3P_{\parallel}$, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, $3P_{\parallel}^{*}$, & '

$\bar{6}m21';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{21}$, S_{3z}, S_{3z}^{-1}, $3P_{\parallel}$, P_z, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, $3L_{21}^{*}$, S_{6z}^{*}, S_{6z}^{-1*}, $3P_{\parallel}^{*}$, C^{*}, & '

$6/m1';L_{21}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, S_{6z}, S_{6z}^{-1}, S_{3z}, S_{3z}^{-1}, P_z, C, $6L_{21}^{*}$, $6P_{\parallel}^{*}$, & '

$\bar{3}m1';L_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, $3L_{21}$, S_{6z}, S_{6z}^{-1}, $3P_{\parallel}$, C, L_{6z}^{*}, L_{6z}^{-1*}, L_{2z}^{*}, $3L_{21}^{*}$, S_{3z}^{*}, S_{3z}^{-1*}, $3P_{\parallel}^{*}$, P_z^{*}. & '

$621';S_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, $6L_{21}$, S_{6z}^{*}, S_{6z}^{-1*}, S_{3z}^{*}, S_{3z}^{-1*}, $6P_{\parallel}^{*}$, P_z^{*}, C^{*}, & '

$6mm1';S_{6z}^{*}$ E, L_{3z}, L_{3z}^{-1}, L_{6z}, L_{6z}^{-1}, L_{2z}, $6P_{\parallel}$, $6L_{21}^{*}$, S_{6z}^{*}, S_{6z}^{-1*}, S_{3z}^{*}, S_{3z}^{-1*}, P_z^{*}, C^{*}, & '

$231';S_{6}^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $4S_6^{*}$, $4S_6^{-1*}$, $3P^{*}$, C^{*}, & '

$231';P^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $6P^{*}$, $3S_4^{*}$, $3S_4^{-1*}$, & '

$231';L_{4}^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $3L_4^{*}$, $3L_4^{-1*}$, $6L_2^{*}$, & '

$431';S_{4}^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $3L_4$, $3L_4^{-1}$, $6L_2$, $3S_4^{*}$, $3S_4^{-1*}$, $4S_6^{*}$, $4S_6^{-1*}$, $6P^{*}$, $3P^{*}$, C^{*}, & '

$\bar{4}3m1';L_{4}^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $3S_4$, $3S_4^{-1}$, $6P$, $3L_4^{*}$, $3L_4^{-1*}$, $6L_2^{*}$, $4S_6^{*}$, $4S_6^{-1*}$, $3P^{*}$, C^{*}, & '

$m31';L_{4}^{*}$ E, $3L_2$, $4L_3$, $4L_3^{-1}$, $4S_6$, $4S_6^{-1}$, $3P$, C, $3L_4^{*}$, $3L_4^{-1*}$, $6L_2^{*}$, $3S_4^{*}$, $3S_4^{-1*}$, $6P^{*}$, & '

Table 21. The Groups of the Set $\{g_p\}$ listed according to their Heesch Subgroup of Order Two

Heesch Group	Groups in $\{g_p\}$ which contain the Heesch Group as a subgroup of Order Two
Triclinic	
1	$1;C^*$ $1;C'^*$ $1;L^*_{2z}$ $1;L'^*_{2z}$ $1;P^*_y$ $1;P'^*_y$
1'	$1';C^*$ $1';L^*_{2z}$ $1';P^*_y$
$\bar{1}$	$\bar{1};L^*_{2y}$ $\bar{1};L'^*_{2y}$
$\bar{1}'$	$\bar{1}';L^*_{2y}$ $\bar{1}';P^*_y$
$\bar{1}1'$	$\bar{1}1';L^*_{2y}$
Monoclinic	
2	$2;P^*_y$ $2;P'^*_y$ $2;L^*_{2x}$ $2;L'^*_{2x}$ $2;P^*_x$ $2;P'^*_x$ $2;L^*_{4z}$ $2;L'^*_{4z}$ $2;S^*_{4z}$ $2;S'^*_{4z}$
2'	$2';P^*_y$ $2';C^*$ $2';L^*_{2z}$ $2';P'^*_x$
21'	$21';P^*_y$ $21';L^*_{2x}$ $21';P^*_x$ $21';L^*_{4z}$ $21';S^*_{4z}$
m	$m;L^*_{2y}$ $m;L'^*_{2y}$ $m;L^*_{2z}$ $m;L'^*_{2z}$
m'	$m';L^*_{2y}$ $m';C^*$ $m';L^*_{2z}$ $m';P^*_y$
ml'	$ml';L^*_{2y}$ $ml';L^*_{2z}$
2/m	$2/m;L^*_{2x}$ $2/m;L'^*_{2x}$ $2/m;L^*_{4z}$ $2/m;L'^*_{4z}$
2'/m	$2'/m;L^*_{2z}$
2/m'	$2/m';L^*_{2x}$ $2/m';L^*_{4z}$ $2/m';S^*_{4z}$ $2/m';P^*_x$
2'/m'	$2'/m';L^*_{2z}$
2/ml'	$2/ml';L^*_{2x}$ $2/ml';L^*_{4z}$

Orthorhombic

222	$222;P_x^*$ $222;P_x'^*$ $222;L_{4z}^*$ $222;L_{4z}'^*$ $222;S_{4z}^*$ $222;S_{4z}'^*$
2'2'2	$2'2'2;P_x^*$ $2'2'2;P_z^*$ $2'2'2;L_{4z}^*$ $2'2'2;S_{4z}^*$ $2'2'2;S_{4z}'^*$
2221'	$2221';P_x^*$ $2221';L_{4z}^*$ $2221';S_{4z}^*$
mm	$mm;L_{2x}^*$ $mm;L_{2x}'^*$ $mm;L_{4z}^*$ $mm;L_{4z}'^*$ $mm;S_{4z}^*$ $mmS_{4z}'^*$
m'm'	$m'm';L_{2x}^*$ $m'm';P_z^*$ $m'm';L_{4z}^*$ $m'm';S_{4z}^*$ $m'm'L_{2xy}^*$ $m'm';L_{4z}'^*$
mm'	$mm';L_{2z}^*$ $mm';C^*$
mml'	$mml';L_{2x}^*$ $mml';L_{4z}^*$ $mml';S_{4z}^*$
mmm	$mmm;L_{4z}^*$ $mmm;L_{4z}'^*$
m'm'm'	$m'm'm';L_{4z}^*$
mmm'	$mmm';L_{4z}^*$ $mmm';S_{4z}^*$
m'm'm	$m'm'm;L_{4z}^*$
mmml'	$mmml';L_{4z}^*$

Tetragonal

4	$4;L_{2x}^*$ $4;L_{2x}'^*$ $4;P_z^*$ $4;P_z'^*$ $4;P_x^*$ $4;P_x'^*$
4'	$4';L_{2x}^*$ $4';P_z^*$ $4';S_{4z}^*$ $4';P_x^*$
41'	$41';L_{2x}^*$ $41';S_{4z}^*$ $41';P_x^*$
42	$42;P_x^*$ $42;P_x'^*$
42'	$42';P_z^*$ $42';P_x^*$
4'2	$4'2;P_x^*$ $4'2;S_{4z}^*$
421'	$421';P_x^*$
4/m	$4/m;L_{2x}^*$ $4/m;L_{2x}'^*$
4/m'	$4/m';L_{2x}^*$ $4/m';P_x^*$

$4'/m$	$4'm;L_{2x}^{*}$
$4'/m'$	$4'/m';P_{x}^{*}$
$4/ml'$	$4/ml';L_{2x}^{*}$
$4mm$	$4mm;L_{2x}^{*}$ $4mm;L_{2x}^{'*}$
$4m'm'$	$4m'm';L_{2x}^{*}$ $4m'm';P_{z}^{*}$
$4'mm'$	$4'mm';L_{2x}^{*}$ $4'mm';S_{4z}^{*}$
$4mml'$	$4mml';L_{2x}^{*}$
$4/mmm$	-
$4/m'm'm'$	-
$4/m'm'm$	-
$4/mmm'$	-
$4'/mmm$	-
$4'/mmm'$	-
$4/mmml'$	-
$\bar{4}$	$\bar{4};L_{4z}^{*}$ $\bar{4};L_{4z}^{'*}$ $\bar{4};P_{x}^{*}$ $\bar{4};P_{x}^{'*}$
$\bar{4}'$	$\bar{4}';L_{4z}^{*}$ $\bar{4}';P_{z}^{*}$ $\bar{4}';L_{2xy}^{*}$ $\bar{4}';P_{x}^{*}$
$\bar{4}1'$	$\bar{4}1';L_{4z}^{*}$ $\bar{4}1';L_{2xy}^{*}$
$\bar{4}2m$	$\bar{4}2m;L_{4z}^{*}$ $\bar{4}2m;L_{4z}^{'*}$
$\bar{4}2m'$	$\bar{4}2m';L_{4z}^{*}$
$\bar{4}'2m'$	$\bar{4}'2m';L_{4z}^{*}$
$\bar{4}'2m$	$\bar{4}'2m;L_{4z}^{*}$ $\bar{4}'2m;L_{2x}^{*}$
$\bar{4}2ml'$	$\bar{4}2ml';L_{4z}^{*}$

Rhombohedral

3	$3;L_{2\perp}^{*}$ $3;L_{2\perp}^{\prime *}$ $3;P_{\parallel}^{*}$ $3;P_{\parallel}^{\prime *}$ $3;S_{6z}^{*}$ $3;S_{6z}^{\prime *}$ $3;S_{3z}^{*}$ $3;S_{3z}^{\prime *}$ $3;L_{6z}^{*}$ $3;L_{6z}^{\prime *}$
$31^{\prime}$	$31^{\prime};L_{3}^{*}$ $31^{\prime};P_{\parallel}^{*}$ $31^{\prime};S_{6z}^{*}$ $31^{\prime};S_{3z}^{*}$ $31^{\prime};L_{6z}^{*}$
32	$32;S_{6z}^{*}$ $32;S_{6z}^{\prime *}$ $32;S_{3z}^{*}$ $32;S_{3z}^{\prime *}$ $32;L_{6z}^{*}$ $32;L_{6z}^{\prime *}$
$32^{\prime}$	$32^{\prime};P_{\parallel}^{*}$ $32^{\prime};S_{6z}^{*}$ $32^{\prime};S_{3z}^{*}$ $32^{\prime};S_{3z}^{\prime *}$ $32^{\prime};L_{6z}^{*}$ $32^{\prime};L_{2\perp}^{*}$
$321^{\prime}$	$321^{\prime};S_{6z}^{*}$ $321^{\prime};S_{3z}^{*}$ $321^{\prime};L_{6z}^{*}$
3m	$3m;S_{6z}^{*}$ $3m;S_{6z}^{\prime *}$ $3m;S_{3z}^{*}$ $3m;S_{3z}^{\prime *}$ $3m;L_{6z}^{*}$ $3m;L_{6z}^{\prime *}$
$3m^{\prime}$	$3m^{\prime};L_{2\perp}^{*}$ $3m^{\prime};S_{6z}^{*}$ $3m^{\prime};S_{3z}^{*}$ $3m^{\prime};S_{3z}^{\prime *}$ $3m^{\prime};L_{6z}^{*}$ $3m^{\prime};P_{\parallel}^{*}$
$3m1^{\prime}$	$3m1^{\prime};S_{6z}^{*}$ $3m1^{\prime};S_{3z}^{*}$ $3m1^{\prime};L_{6z}^{*}$
$\bar{3}$	$\bar{3};P_{\parallel}^{*}$ $\bar{3};P_{\parallel}^{\prime *}$ $\bar{3};L_{6z}^{*}$ $\bar{3};L_{6z}^{\prime *}$
$\bar{3}^{\prime}$	$\bar{3}^{\prime};L_{2\perp}^{*}$ $\bar{3}^{\prime};P_{\parallel}^{*}$ $\bar{3}^{\prime};S_{3z}^{*}$ $\bar{3}^{\prime};L_{6z}^{*}$
$\bar{3}1^{\prime}$	$\bar{3}1^{\prime};L_{2\perp}^{*}$ $\bar{3}1^{\prime};L_{6z}^{*}$
$\bar{3}m$	$\bar{3}m;L_{6z}^{*}$ $\bar{3}m;L_{6z}^{\prime *}$
$\bar{3}^{\prime}m^{\prime}$	$\bar{3}^{\prime}m^{\prime};S_{3z}^{*}$ $\bar{3}^{\prime}m^{\prime};L_{6z}^{*}$
$\bar{3}^{\prime}m$	$\bar{3}^{\prime}m;S_{3z}^{*}$ $\bar{3}^{\prime}m;L_{6z}^{*}$
$\bar{3}m^{\prime}$	$\bar{3}m^{\prime};L_{6z}^{*}$ $\bar{3}m^{\prime};L_{2\perp}^{*}$
$\bar{3}m1^{\prime}$	$\bar{3}m1^{\prime};L_{6z}^{*}$

Hexagonal

$\bar{6}$	$\bar{6};L_{2\perp}^{*}$ $\bar{6};L_{2\perp}^{\prime *}$ $\bar{6};L_{6z}^{*}$
$\bar{6}^{\prime}$	$\bar{6}^{\prime};P_{\parallel}^{*}$ $\bar{6}^{\prime};L_{2\perp}^{*}$ $\bar{6}^{\prime};L_{6z}^{*}$ $\bar{6}^{\prime};S_{6z}^{*}$
$\bar{6}1^{\prime}$	$\bar{6}1^{\prime};L_{2\perp}^{*}$ $\bar{6}1^{\prime};L_{6z}^{*}$
$\bar{6}m2$	$\bar{6}m2;L_{6z}^{*}$ $\bar{6}m2;L_{6z}^{\prime *}$

$\bar{6}m'2'$	$\bar{6}m'2';L^*_{2\perp}$ $\bar{6}m'2';L^*_{6z}$
$\bar{6}'m2'$	$\bar{6}'m2';S^*_{6z}$ $\bar{6}'m2';L^*_{6z}$
$\bar{6}'m'2$	$\bar{6}'m'2;S^*_{6z}$ $\bar{6}'m'2;L^*_{6z}$
$\bar{6}m21'$	$\bar{6}m21';L^*_{6z}$
6	$6;L^*_{2\perp}$ $6;L'^*_{2\perp}$ $6;S^*_{6z}$ $6;L'^*_{6z}$ $6;S'^*_{6z}$ $6;P^*_{\parallel}$ $6;P'^*_{\parallel}$
6'	$6';L^*_{2\perp}$ $6';S^*_{3z}$ $6';S^*_{6z}$ $6';P^*_{\parallel}$
61'	$61';L^*_{2\perp}$ $61';S^*_{6z}$ $61';P^*_{\parallel}$
62	$62;S^*_{6z}$ $62;S'^*_{6z}$
62'	$62';P^*_{\parallel}$ $62';S^*_{6z}$
6'2	$6'2;S^*_{3z}$ $6'2;S^*_{6z}$
621'	$621';S^*_{6z}$
6/m	$6/m;L^*_{2\perp}$ $6/m;L'^*_{2\perp}$
6'/m	$6'/m;L^*_{2\perp}$
6/m'	$6/m';L^*_{2\perp}$ $6/m';P^*_{\parallel}$
6'/m'	$6'/m';L^*_{2\perp}$
6/m1'	$6/m1';L^*_{2\perp}$
6mm	$6mm;S^*_{6z}$ $6mm;L'^*_{2\perp}$
6m'm'	$6m'm';S^*_{6z}$ $6m'm';L^*_{2\perp}$
6'm'm	$6'm'm;S^*_{3z}$ $6'm'm;S^*_{6z}$
6mm1'	$6mm1';S^*_{6z}$
6/mm	-
6'/mm	-
6/mm'	-
6'/m'm	-
6/m'm'	-
6/m'm	-
6/mm1'	-

Cubic

23	$23;S_6^*$ $23;S_6'^*$ $23;P^*$ $23;P'^*$ $23;L_4^*$ $23;L_4'^*$
$231'$	$231';S_6^*$ $231';S_4^*$ $231';L_4^*$
$m3$	$m3;L_4^*$ $m3;L_4'^*$
$m'3$	$m'3;L_4^*$ $m'3;S_4^*$
$m31'$	$m31';L_4^*$
$\bar{4}3m$	$\bar{4}3m;L_4^*$ $\bar{4}3m;L_4'^*$
$\bar{4}3m'$	$\bar{4}3m';L_4^*$ $\bar{4}3m';S_6^*$
$\bar{4}3ml'$	$\bar{4}3ml';L_4^*$
43	$43;S_4^*$ $43;S_4'^*$
$4'3$	$4'3;S_4^*$ $4'3;S_6^*$
$431'$	$431';S_4^*$
$m3m$	-
$m'3m'$	-
$m3m'$	-
$m'3m'$	-
$m3ml'$	-

Table 22. The Possible Merohedry Twin Groups

Heesch Group	Possible Merohedry Twin Groups
Triclinic	
1	$1;C^*$ $1;C'^*$
1'	$1';C^*$
$\bar{1}$	-
$\bar{1}'$	-
$\bar{1}1'$	-
Monoclinic	
2	$2;P_y^*$ $2;P_y'^*$
2'	$2';P_y^*$ $2';C^*$
21'	$21';P_y^*$
m	$m;L_{2y}^*$ $m;L_{2y}'^*$
m'	$m';L_{2y}^*$ $m';C^*$
m1'	$m1';L_{2y}^*$
2/m	-
2'/m	-
2/m'	-
2'/m'	-
2/m1'	-

Orthorhombic

222	$222;P_x^*$ $222;P_x'^*$
$2'2'2$	$2'2'2;P_x^*$ $2'2'2;P_z^*$
$2221'$	$2221';P_x^*$
mm	$mm;L_{2x}^*$ $mm;L_{2x}'^*$
$m'm'$	$m'm';L_{2x}^*$ $m'm';P_z^*$
mm'	$mm';L_{2z}^*$ $mm';C^*$
$mm1'$	$mm1';L_{2x}^*$
mmm	-
$m'm'm'$	-
mmm'	-
$m'm'm$	-
$mmm1'$	-

Tetragonal

4	$4;L_{2x}^*$ $4;L_{2x}'^*$ $4;P_z^*$ $4;P_z'^*$ $4;P_x^*$ $4;P_x'^*$
$4'$	$4';L_{2x}^*$ $4';P_z^*$ $4';S_{4z}^*$ $4';P_x^*$
$41'$	$41';L_{2x}^*$ $41';S_{4z}^*$ $41';P_x^*$
42	$42;P_x^*$ $42;P_x'^*$
$42'$	$42';P_z^*$ $42';P_x^*$
$4'2$	$4'2;P_x^*$ $4'2;S_{4z}^*$
$421'$	$421';P_x^*$
4/m	$4/m;L_{2x}^*$ $4/m;L_{2x}'^*$
$4/m'$	$4/m';L_{2x}^*$ $4/m';P_x^*$
$4'/m$	$4'/m;L_{2x}^*$
$4'/m'$	$4'/m';P_x^*$
$4/m1'$	$4/m1';L_{2x}^*$

4mm	$4mm;L^{*}_{2x}$	$4mm;L^{'*}_{2x}$			
4m'm'	$4m'm';L^{*}_{2x}$	$4m'm';P^{*}_{z}$			
4'mm'	$4'mm';L^{*}_{2x}$	$4'mm';S^{*}_{4z}$			
4mm1'	$4mm1';L^{*}_{2x}$				
4/mmm	-				
4/m'm'm'	-				
4/m'm'm	-				
4/mmm'	-				
4'/mmm	-				
4'/mmm'	-				
4/mmm1'	-				
$\bar{4}$	$\bar{4};L^{*}_{4z}$	$\bar{4};L^{'*}_{4z}$	$\bar{4};P^{*}_{x}$	$\bar{4};P^{'*}_{x}$	
$\bar{4}'$	$\bar{4}';L^{*}_{4z}$	$\bar{4}';P^{*}_{z}$	$\bar{4}';L^{*}_{2xy}$	$\bar{4}';P^{*}_{x}$	
$\bar{4}1'$	$\bar{4}1';L^{*}_{4z}$	$\bar{4}1';L^{*}_{2xy}$			
$\bar{4}2m$	$\bar{4}2m;L^{*}_{4z}$	$\bar{4}2m;L^{'*}_{4z}$			
$\bar{4}2m'$	$\bar{4}2m';L^{*}_{4z}$				
$\bar{4}'2m'$	$\bar{4}'2m';L^{*}_{4z}$				
$\bar{4}'2m$	$\bar{4}'2m;L^{*}_{4z}$	$\bar{4}'2m;L^{*}_{2x}$			
$\bar{4}2m1'$	$\bar{4}2m1';L^{*}_{4z}$				

Rhombohedral

3	$3;L^{*}_{2\perp}$	$3;L^{'*}_{2\perp}$	$3;P^{*}_{\parallel}$	$3;P^{'*}_{\parallel}$	$3;S^{*}_{6z}$	$3;S^{'*}_{6z}$
31'	$31';L^{*}_{2\perp}$	$31';P^{*}_{\parallel}$	$31';S^{*}_{6z}$			
32	$32;S^{*}_{6z}$	$32;S^{'*}_{6z}$				
32'	$32';P^{*}_{\parallel}$	$32';S^{*}_{6z}$				
321'	$321';S^{*}_{6z}$					
3m	$3m;S^{*}_{6z}$	$3m;S^{'*}_{6z}$				
3m'	$3m';L^{*}_{2\perp}$	$3m';S^{*}_{6z}$				

$3m1'$	$3m1';S^*_{6z}$
$\bar{3}$	$\bar{3};P^*_{\parallel}$ $\bar{3};P^{'*}_{\parallel}$
$\bar{3}'$	$\bar{3}';L^*_{2\perp}$ $\bar{3}';P^*_{\parallel}$
$\bar{3}1'$	$\bar{3}1';L^*_{2\perp}$
$\bar{3}m$	-
$\bar{3}'m'$	-
$\bar{3}'m$	-
$\bar{3}m'$	-
$\bar{3}m1'$	-

Hexagonal

$\bar{6}$	$\bar{6};L^*_{2\perp}$ $\bar{6};L^{'*}_{2\perp}$ $\bar{6};L^*_{6z}$
$\bar{6}'$	$\bar{6}';P^*_{\parallel}$ $\bar{6}';L^*_{2\perp}$ $\bar{6}';L^*_{6z}$ $\bar{6}';S^*_{6z}$
$\bar{6}1'$	$\bar{6}1';L^*_{2\perp}$ $\bar{6}1';L^*_{6z}$
$\bar{6}m2$	$\bar{6}m2;L^*_{6z}$ $\bar{6}m2;L^{'*}_{6z}$
$\bar{6}m'2'$	$\bar{6}m'2';L^*_{2\perp}$ $\bar{6}m'2';L^*_{6z}$
$\bar{6}'m2'$	$\bar{6}'m2';S^*_{6z}$ $\bar{6}'m2';L^*_{6z}$
$\bar{6}'m'2$	$\bar{6}'m'2;S^*_{6z}$ $\bar{6}'m'2;L^*_{6z}$
$\bar{6}m21'$	$\bar{6}m21';L^*_{6z}$
6	$6;L^*_{2\perp}$ $6;L^{'*}_{2\perp}$ $6;S^*_{6z}$ $6;L^{'*}_{6z}$ $6;S^{'*}_{6z}$ $6;P^*_{\parallel}$ $6;P^{'*}_{\parallel}$
$6'$	$6';L^*_{2\perp}$ $6';S^*_{3z}$ $6';S^*_{6z}$ $6';P^*_{\parallel}$
$61'$	$61';L^*_{2\perp}$ $61';S^*_{6z}$ $61';P^*_{\parallel}$
62	$62;S^*_{6z}$ $62;S^{'*}_{6z}$
$62'$	$62';P^*_{\parallel}$ $62';S^*_{6z}$
$6'2$	$6'2;S^*_{3z}$ $6'2;S^*_{6z}$
$621'$	$621';S^*_{6z}$
$6/m$	$6/m;L^*_{2\perp}$ $6/m;L^{'*}_{2\perp}$

$6'/m$	$6'/m;L_{2\perp}^{*}$
$6/m'$	$6/m';L_{2\perp}^{*}$ $6/m';P_{\parallel}^{*}$
$6'/m'$	$6'/m';L_{2\perp}^{*}$
$6/ml'$	$6/ml';L_{2\perp}^{*}$
$6mm$	$6mm;S_{6z}^{*}$ $6mm;L_{2\perp}^{'*}$
$6m'm'$	$6m'm';S_{6z}^{*}$ $6m'm';L_{2\perp}^{*}$
$6'm'm$	$6'm'm;S_{3z}^{*}$ $6'm'm;S_{6z}^{*}$
$6mml'$	$6mml';S_{6z}^{*}$
$6/mm$	-
$6'/mm$	-
$6/mm'$	-
$6'/m'm$	-
$6/m'm'$	-
$6/m'm$	-
$6/mml'$	-

Cubic

23	$23;S_{6}^{*}$ $23;S_{6}^{'*}$ $23;P^{*}$ $23;P^{'*}$ $23;L_{4}^{*}$ $23;L_{4}^{'*}$
$231'$	$231';S_{6}^{*}$ $231';P^{*}$ $231';L_{4}^{*}$
$m3$	$m3;L_{4}^{*}$ $m3;L_{4}^{'*}$
$m'3$	$m'3;L_{4}^{*}$ $m'3;S_{4}^{*}$
$m31'$	$m31';L_{4}^{*}$
$\bar{4}3m$	$\bar{4}3m;L_{4}^{*}$ $\bar{4}3m;L_{4}^{'*}$
$\bar{4}3m'$	$\bar{4}3m';L_{4}^{*}$ $\bar{4}3m';S_{6}^{*}$
$\bar{4}3ml'$	$\bar{4}3ml';L_{4}^{*}$
43	$43;S_{4}^{*}$ $43;S_{4}^{'*}$
$4'3$	$4'3;S_{4}^{*}$ $4'3;S_{6}^{*}$

$431'$	$431';S_4^*$
$m3m$	-
$m^{\dagger}3m'$	-
$m3m'$	-
$m'3m'$	-
$m3ml'$	-

Table 23. The Possible Reticular Merohedry Twin Groups for Rhombohedral Crystals

Heesch Group	Possible Reticular Merohedry Twin Groups
3	$3;L^{*}_{2\perp}$ $3;L^{'*}_{2\perp}$ $3;P^{*}_{\parallel}$ $3;P^{'*}_{\parallel}$ $3;S^{*}_{3z}$ $3;S^{'*}_{3z}$ $3;L^{*}_{6z}$ $3;L^{'*}_{6z}$
31'	$31';L^{*}_{2\perp}$ $31';P^{*}_{\parallel}$ $31';S^{*}_{3z}$ $31';L^{*}_{6z}$
32	$32;S^{*}_{3z}$ $32;S^{'*}_{3z}$ $32;L^{*}_{6z}$ $32;L^{'*}_{6z}$
32'	$32';S^{*}_{3z}$ $32';S^{'*}_{3z}$ $32';L^{*}_{6z}$ $32';L^{*}_{2\perp}$
321'	$321';S^{*}_{3z}$ $321';L^{*}_{6z}$
3m	$3m;S^{*}_{3z}$ $3m;S^{'*}_{3z}$ $3m;L^{*}_{6z}$ $3m;L^{'*}_{6z}$
3m'	$3m';S^{*}_{3z}$ $3m';S^{'*}_{3z}$ $3m';L^{*}_{6z}$ $3m';P^{*}_{\parallel}$
3ml'	$3ml';S^{*}_{3z}$ $3ml';L^{*}_{6z}$
$\bar{3}$	$\bar{3};P^{*}_{\parallel}$ $\bar{3};P^{'*}_{\parallel}$ $\bar{3};L^{*}_{6z}$ $\bar{3};L^{'*}_{6z}$
$\bar{3}'$	$\bar{3}';L^{*}_{2\perp}$ $\bar{3}';P^{*}_{\parallel}$ $\bar{3}';S^{*}_{3z}$ $\bar{3}';L^{*}_{6z}$
$\bar{3}1'$	$\bar{3}1';L^{*}_{2\perp}$ $\bar{3}1';L^{*}_{6z}$
$\bar{3}m$	$\bar{3}m;L^{*}_{6z}$ $\bar{3}m;L^{'*}_{6z}$
$\bar{3}'m'$	$\bar{3}'m';S^{*}_{3z}$ $\bar{3}'m';L^{*}_{6z}$
$\bar{3}'m$	$\bar{3}'m;S^{*}_{3z}$ $\bar{3}'m;L^{*}_{6z}$
$\bar{3}m'$	$\bar{3}m';L^{*}_{6z}$ $\bar{3}m';L^{*}_{2\perp}$
$\bar{3}ml'$	$\bar{3}ml';L^{*}_{6z}$

Table 24. The Possible Reticular Merohedry Twin Groups for Cubic Crystals

Heesch Group	Possible Reticular Merohedry Twin Groups
23	$23,3;L^{*}_{2\perp}$ $23,3;L^{'*}_{2\perp}$ $23,3;P^{*}_{\parallel}$ $23,3;P^{'*}_{\parallel}$ $23,3;S^{*}_{3z}$ $23,3;S^{'*}_{3z}$ $23,3;L^{*}_{6z}$ $23,3;L^{'*}_{6z}$
231'	$231',31';L^{*}_{2\perp}$ $231',31';P^{*}_{\parallel}$ $231',31';S^{*}_{3z}$ $231',31';L^{*}_{6z}$
m3	$m3,\bar{3};P^{*}_{\parallel}$ $m3,\bar{3};P^{'*}_{\parallel}$ $m3,\bar{3};L^{*}_{6z}$ $m3,\bar{3};L^{'*}_{6z}$
m'3	$m'3,\bar{3}';L^{*}_{2\perp}$ $m'3,\bar{3}';P^{*}_{\parallel}$ $m'3,\bar{3}';S^{*}_{3z}$ $m'3,\bar{3}';L^{*}_{6z}$
m31'	$m31',\bar{3}1';L^{*}_{2\perp}$ $m31',\bar{3}1';L^{*}_{6z}$
$\bar{4}3m$	$\bar{4}3m,3m;S^{*}_{3z}$ $\bar{4}3m,3m;S^{'*}_{3z}$ $\bar{4}3m,3m;L^{*}_{6z}$ $\bar{4}3m,3m;L^{'*}_{6z}$
$\bar{4}3m'$	$\bar{4}3m',3m';S^{*}_{3z}$ $\bar{4}3m',3m';S^{'*}_{3z}$ $\bar{4}3m',3m';L^{*}_{6z}$ $\bar{4}3m,3m';P^{*}_{\parallel}$
$\bar{4}3m1'$	$\bar{4}3m1',3m1';S^{*}_{3z}$ $\bar{4}3m1',3m1';L^{*}_{6z}$
43	$43,32;S^{*}_{3z}$ $43,32;S^{'*}_{3z}$ $43,32;L^{*}_{6z}$ $43,32;L^{'*}_{6z}$
4'3	$4'3,32';S^{*}_{3z}$ $4'3,32';S^{'*}_{3z}$ $4'3,32';L^{*}_{6z}$ $4'3,32';L^{*}_{2\perp}$
431'	$431',321';S^{*}_{3z}$ $431',321';L^{*}_{6z}$
m3m	$m3m,\bar{3}m;L^{*}_{6z}$ $m3m,\bar{3}m;L^{'*}_{6z}$
m'3m'	$m'3m',\bar{3}'m';S^{*}_{3z}$ $m'3m',\bar{3}'m';L^{*}_{6z}$
m3m'	$m3m',\bar{3}'m;S^{*}_{3z}$ $m3m',\bar{3}'m;L^{*}_{6z}$
m'3m'	$m'3m',\bar{3}\,m',\bar{3}m';L^{*}_{6z}$ $m'3m',\bar{3}m';L^{*}_{2\perp}$
m3m1'	$m3m1',\bar{3}m1';L^{*}_{6z}$

Appendix

Let $\underline{H}$ be the total magnetic field at the proton site. Then the Hamiltonian $\mathcal{H}$ for the proton may be written as

$$\mathcal{H} = -g\beta \underline{I} \cdot \underline{H}$$

where g is the gyromagnetic ratio, β the nuclear magneton $e\hbar/2Mc$ and $\underline{I}$ the total nuclear angular momentum in units of $\hbar$. Then

$$\underline{I} \cdot \underline{H} = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} H_x + \begin{pmatrix} 0 & -i\frac{1}{2} \\ i\frac{1}{2} & 0 \end{pmatrix} H_y + \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} H_z$$

$$= \frac{1}{2} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix}.$$

Let $H_z \equiv H_0 + H_{11}$ where H_0 is the applied dc field and H_{11} is the z component of the local field H_ℓ. Then $\mathcal{H}\psi = E\psi$ and

$$\begin{vmatrix} H_z + \frac{2E}{g\beta} & H_x - iH_y \\ H_x + iH_y & -H_z + \frac{2E}{g\beta} \end{vmatrix} = 0.$$

$$\therefore E = \pm \frac{g\beta}{2} \sqrt{(H_0 + H_{11})^2 + (H_x^2 + H_y^2)} \quad \text{and}$$

$$h\nu = \Delta E = g\beta \sqrt{H_0^2 + 2H_0 H_{11} + H_\ell^2}\,.$$

Let $h\nu_0 = g\beta H_0$. Then since $H_{11} = H_\ell \cos\Theta$,

$$\frac{\nu - \nu_0}{\nu_0} = \sqrt{1 + \left(\frac{H_\ell}{H_0}\right)^2 + 2\frac{H_\ell}{H_0}\cos\Theta} \quad - 1.$$

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