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Volume E

SUBPERIODIC GROUPS

Edited by

V. KOPSKÝ AND D. B. LITVIN

Dedicated to

Mary

V. KOPSKÝ

Tikva (זכרונה לברכה) and Professor W. Opechowski,
may their memories be blessed.

D. B. LITVIN

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Preface

BY V. KOPSKÝ AND D. B. LITVIN

This volume is divided into two sections. The first, covered in Parts 1–4, can be considered as an extension of Volume A: *Space-Group Symmetry*, in this series of *International Tables for Crystallography*. As Volume A treats one-, two-, and three-dimensional space groups, this Volume treats the two- and three-dimensional subperiodic groups. That is, it treats the frieze groups, two-dimensional groups with one-dimensional translations, the rod groups, three-dimensional groups with one-dimensional translations, and layer groups, three-dimensional groups with two-dimensional translations. A reader familiar with Volume A should readily recognize the format and content of the tables of Parts 1–4 of this volume. The information presented about the subperiodic groups is in the same format and consists of the same content as that provided in Volume A for space groups.

A relationship between space and subperiodic groups is considered in Parts 5 and 6: given a crystal of a specific space-group symmetry and a plane transecting the crystal, one can enquire as to what is the layer subgroup of the space group which leaves this plane invariant. The physical motivation for answering this question is discussed in Chapter 5.2. This is followed by the 'Scanning Tables' in which the layer symmetries of 'sectional' planes are tabulated for all crystallographic orientations and for all positions (locations) of these planes. These tables also contain explicitly the orbits of these planes and implicitly, *via* the so-called 'scanning groups', information about the rod symmetries of straight lines which penetrate through the crystal.

The history of this work dates back to 1972 when one of us (DBL) was asked by a fellow post doc, John Berlinsky, if there existed International-like tables to classify arrays of hydrogen molecules on a surface with the molecules not constrained to be 'in-plane'. Tables for the layer groups were subsequently derived in the content and format of the *International Tables for X-ray Crystallography*, Volume 1 (1952). It was later pointed out by a referee of *Acta Crystallographica* that such tables had already been published by E. Wood in 1964. Work on these tables remained dormant until 1983 with the publication of Volume A of the *International Tables for Crystallography*, and the extensive addition of new features in the description of each space group. Work began then on including these new features into tables for the layer groups.

During this same time one of us (VK) was asked by Dr V. Janovec to investigate the group theoretical aspects of the analysis of domain walls and twin boundaries. Thus, work began on the relationships between space groups and subperiodic groups and standards for the subperiodic groups.

It is our subsequent collaboration which has led to the material presented in this volume. In the many decisions concerning the choice of symbols, origins, and settings for the subperiodic groups, the final choices were made based on relationships between space groups and subperiodic groups. While these relationships are not all explicitly given here, they have been implicitly used.

As to the dedication, we would like to point out, to quell any rumors to the contrary, that Mary and Tikva (זכרונה לברכה) are our respective wives. Their unending patience and constant encouragement are indeed due recognition. The parenthetical Hebrew means 'may her memory be blessed', and Professor W. Opechowski is included as DBL's scientific 'father'.

1.2. Guide to the use of the subperiodic group tables

This present volume is, in part, an extension of *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 1983). Symmetry tables are given in *IT* A for the 230 three-dimensional crystallographic space-group types (space groups) and the 17 two-dimensional crystallographic space-group types (plane groups). We give in the following three parts of this volume analogous symmetry tables for the two-dimensional and three-dimensional subperiodic group types: the seven crystallographic *frieze-group* types (two-dimensional groups with one-dimensional translations) in Part 2; the 75 crystallographic *rod-group* types (three-dimensional groups with one-dimensional translations) in Part 3; and the 80 crystallographic *layer-group* types (three-dimensional groups with two-dimensional translations) in Part 4. This chapter forms a guide to the entries of the subperiodic group tables given in Parts 2–4.

1.2.1. Classification of subperiodic groups

Subperiodic groups can be classified in ways analogous to the space groups. For the mathematical definitions of these classifications and their use for space groups, see Section 8.2 of *IT* A (1983). Here we shall limit ourselves to those classifications which are explicitly used in the symmetry tables of the subperiodic groups.

1.2.1.1. *Subperiodic group types*

The subperiodic groups are classified into *affine subperiodic group types*, *i.e.* affine equivalence classes of subperiodic groups. There are 80 affine layer-group types and seven affine frieze-group types. There are 67 crystallographic and an infinity of noncrystallographic affine rod-group types. We shall consider here only rod groups of the 67 crystallographic rod-group types and refer to these crystallographic affine rod-group types simply as affine rod-group types.

The subperiodic groups are also classified into *proper affine subperiodic group types*, *i.e.* proper affine classes of subperiodic groups. For layer and frieze groups, the two classifications are identical. For rod groups, each of eight affine rod-group types splits into a pair of *enantiomorphic crystallographic rod-group types*. Consequently, there are 75 proper affine rod-group types. The eight pairs of enantiomorphic rod-group types are $p4_1$ (R24), $p4_3$ (R26); $p4_122$ (R31), $p4_322$ (R33); $p3_1$ (R43), $p3_2$ (R44); $p3_112$ (R47), $p3_212$ (R48); $p6_1$ (R54), $p6_5$ (R58); $p6_2$ (R55), $p6_4$ (R57); $p6_122$ (R63), $p6_522$ (R67); and $p6_222$ (R64), $p6_422$ (R66). (Each subperiodic group is given in the text by its Hermann–Mauguin symbol followed in parenthesis by a letter L, R or F to denote it, respectively, as a layer, rod or frieze group, and its sequential numbering from Parts 2, 3 or 4.) We shall refer to the proper affine subperiodic group types simply as subperiodic group types.

1.2.1.2. *Other classifications*

There are 27 geometric crystal classes of layer groups and rod groups, and four geometric crystal classes of frieze groups. These are listed, for layer groups, in the fourth column of Table 1.2.1.1, and for the rod and frieze groups in the second columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

We further classify subperiodic groups according to the following classifications of the subperiodic group's point group and lattice group. These classifications are introduced to emphasize the relationships between subperiodic groups and space groups:

(1) The point group of a layer or rod group is three-dimensional and corresponds to a point group of a three-dimensional space group. The point groups of three-dimensional space groups are classified into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic crystal systems. We shall use this classification also for subperiodic groups. Consequently, the three-dimensional subperiodic groups are classified, see the third column of Table 1.2.1.1 and the first column of Table 1.2.1.2, into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal crystal systems. The cubic crystal system does not arise for three-dimensional subperiodic groups. Two-dimensional subperiodic groups, *i.e.* frieze groups, are analogously classified, see the first column of Table 1.2.1.3, into the oblique and rectangular crystal systems.

(2) The two-dimensional lattice of a layer group is also a two-dimensional lattice of a plane group. The lattices of plane groups are classified, according to *Bravais* (*flock*) *systems*, see *IT* A (1983), into the oblique, rectangular, square and hexagonal Bravais systems. We shall also use this classification for layer groups, see the first column in Table 1.2.1.1. For rod and frieze groups no lattice classification is used, as all one-dimensional lattices form a single Bravais system.

A subdivision of the monoclinic rod-group category is made into monoclinic/inclined and monoclinic/orthogonal. Two different coordinate systems, see Table 1.2.1.2, are used for the rod groups of these two subdivisions of the monoclinic crystal system. These two coordinate systems differ in the orientation of the plane containing the non-lattice basis vectors relative to the lattice vectors. For the monoclinic/inclined subdivision, the plane containing the non-lattice basis vectors is, see Fig. 1.2.1.1, *inclined* with respect to the lattice basis vector. For the monoclinic/orthogonal subdivision, the plane is, see Fig. 1.2.1.2, *orthogonal*.

1.2.1.2.1. *Conventional coordinate systems*

The subperiodic groups are described by means of a *crystallographic coordinate system* consisting of a *crystallographic origin*, denoted by *O*, and a *crystallographic basis*. The basis vectors for the three-dimensional layer groups and rod groups are labelled **a**, **b** and **c**. The basis vectors for the two-dimensional frieze groups are labelled **a** and **b**. Unlike space groups, not all basis vectors of the crystallographic basis are lattice vectors. Like space groups, the crystallographic coordinate system is used to define the symmetry operations (see Section 1.2.9) and the Wyckoff positions (see Section 1.2.11). The symmetry operations are defined with respect to the directions of both lattice and non-lattice basis vectors. A Wyckoff position, denoted by a coordinate triplet (x, y, z) for the three-dimensional layer and rod groups, is defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$. For the two-dimensional frieze groups, a Wyckoff position is denoted by a coordinate doublet (x, y) and is defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b}$.

The term *setting* will refer to the assignment of the labels **a**, **b** and **c** (and the corresponding directions [100], [010] and [001], respectively) to the basis vectors of the crystallographic basis (see Section 1.2.6). In the *standard setting*, those basis vectors which are also lattice vectors are labelled as follows: for layer groups with their two-dimensional lattice by **a** and **b**, for rod groups with

No. 7 $p2mg$ Patterson symmetry $p2mm$

p_a2mg

p_b2gm
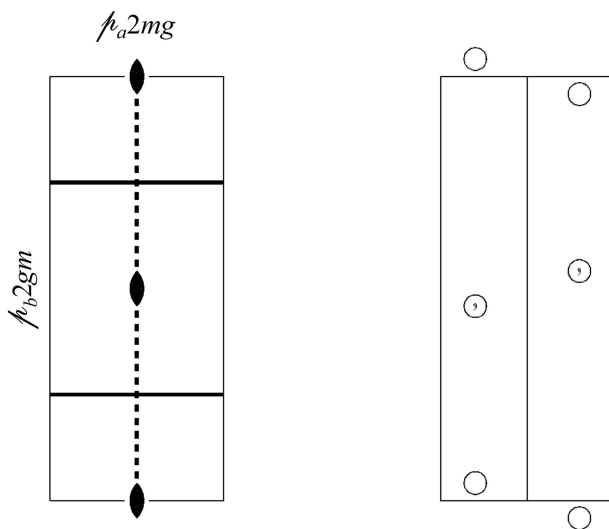
Origin at $2\,1\,g$

Asymmetric unit $0 \le x \le \frac{1}{4}$

Symmetry operations

(1) 1   (2) 2   0,0   (3) m $\frac{1}{4},y$ (4) g $x,0$

Generators selected   (1); $t(1)$; (2); (3)

Positions

Multiplicity,   Coordinates   Reflection conditions
Wyckoff letter,
Site symmetry   General:

4   c 1   (1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x}+\frac{1}{2},y$ (4) $x+\frac{1}{2},\bar{y}$ $h \;:\; h = 2n$

                                                                 Special: no extra conditions

2   b $.m.$ $\frac{1}{4},y$ $\frac{3}{4},\bar{y}$

2   a $2..$ $0,0$ $\frac{1}{2},0$

Symmetry of special projections
Along $[10]$ m Along $[01]$ pm
                                                   $\mathbf{a}' = \frac{1}{2}\mathbf{a}$
Origin at $x,0$ Origin at $0,y$

Maximal non-isotypic subgroups
I $[2]\,p11g\,(5)$ 1; 4
        $[2]\,p1m1\,(3)$ 1; 3
        $[2]\,p211\,(2)$ 1; 2
IIa   none
IIb   none

Maximal isotypic subgroups of lowest index
IIc $[3]\,p2mg\,(\mathbf{a}' = 3\mathbf{a})\,(7)$

Minimal non-isotypic supergroups
I   none
II $[2]\,p2mm\,(\mathbf{a}' = \frac{1}{2}\mathbf{a})\,(6)$
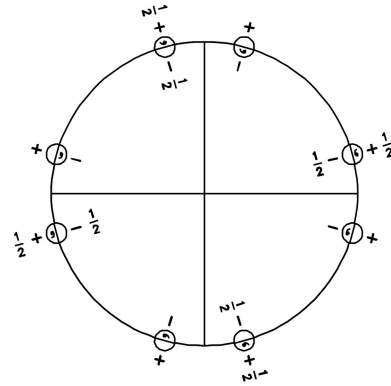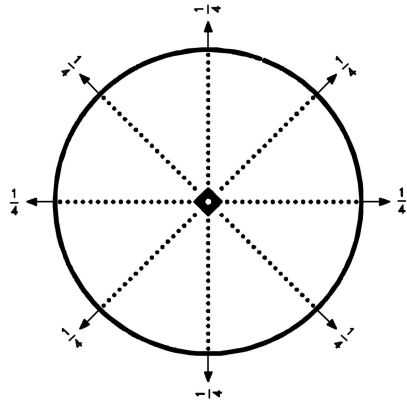
Origin at centre $(4/m)$ at $4/mcc$

Asymmetric unit $0 \le x;$ $0 \le y;$ $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,\frac{1}{4}$	(6) 2 $x,0,\frac{1}{4}$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) c $x,0,z$	(14) c $0,y,z$	(15) c $x,\bar{x},z$	(16) c x,x,z

Generators selected (1); $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions

16   g 1

(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$
(5) $\bar{x},y,\bar{z}+\frac{1}{2}$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
(9) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$
(13) $x,\bar{y},z+\frac{1}{2}$ (14) $\bar{x},y,z+\frac{1}{2}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$ (16) $y,x,z+\frac{1}{2}$

General:

l : $l=2n$

Special: no extra conditions

8   f m . .
$x,y,0$ $\bar{x},\bar{y},0$ $\bar{y},x,0$ $y,\bar{x},0$
$\bar{x},y,\frac{1}{2}$ $x,\bar{y},\frac{1}{2}$ $y,x,\frac{1}{2}$ $\bar{y},\bar{x},\frac{1}{2}$

8   e . 2 .
$x,0,\frac{1}{4}$ $\bar{x},0,\frac{1}{4}$ $0,x,\frac{1}{4}$ $0,\bar{x},\frac{1}{4}$
$\bar{x},0,\frac{3}{4}$ $x,0,\frac{3}{4}$ $0,\bar{x},\frac{3}{4}$ $0,x,\frac{3}{4}$

8   d . . 2
$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{1}{4}$ $x,\bar{x},\frac{1}{4}$
$\bar{x},\bar{x},\frac{3}{4}$ $x,x,\frac{3}{4}$ $x,\bar{x},\frac{3}{4}$ $\bar{x},x,\frac{3}{4}$

4   c 4 . .
$0,0,z$ $0,0,\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$ $0,0,z+\frac{1}{2}$

2   b $4/m$ . .
$0,0,0$ $0,0,\frac{1}{2}$

2   a 4 2 2
$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$

Symmetry of special projections

Along [001] $4mm$

Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isotypic non-enantiomorphic subgroups

I   [2]$p\bar{4}2c$ (38)   1; 2; 5; 6; 11; 12; 15; 16
     [2]$p\bar{4}c2$ ($p\bar{4}2c$, 38)   1; 2; 7; 8; 11; 12; 13; 14
     [2]$p4cc$ (36)   1; 2; 3; 4; 13; 14; 15; 16
     [2]$p422$ (30)   1; 2; 3; 4; 5; 6; 7; 8
     [2]$p4/m11$ ($p4/m$, 28)   1; 2; 3; 4; 9; 10; 11; 12
     [2]$p2/m2/c1$ ($pccm$, 21)   1; 2; 5; 6; 9; 10; 13; 14
     [2]$p2/m12/c$ ($pccm$, 21)   1; 2; 7; 8; 9; 10; 15; 16

IIa   none
IIb   none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc   [3]$p4/mcc$ ($\mathbf{c}' = 3\mathbf{c}$) (40)

Minimal non-isotypic non-enantiomorphic supergroups

I   none
II   [2]$p4/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (39)

ORIGIN CHOICE 1
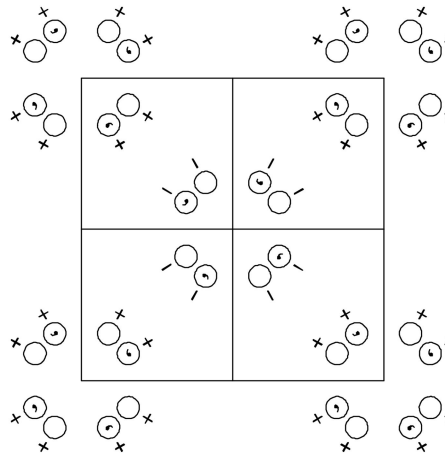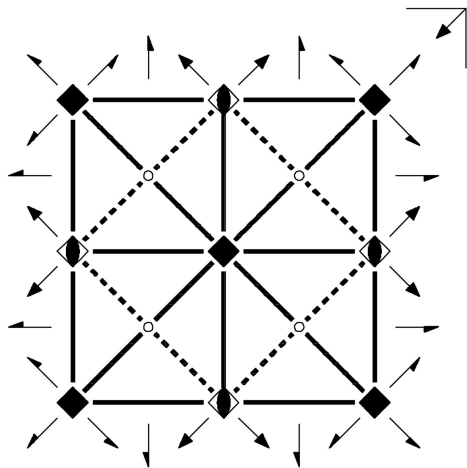
Origin on $4mm$ at $-\frac{1}{4}, -\frac{1}{4}, 0$ from centre $(2/m)$

Asymmetric unit $\qquad$ $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad y \le \frac{1}{2} - x; \quad 0 \le z$

Symmetry operations

(1) 1

(2) 2 $\quad 0,0,z$

(3) 4^+ $0,0,z$

(4) 4^- $\ 0,0,z$

(5) $2(\frac{1}{2},\frac{1}{2},0)$ $\ \ 0,y,0$

(6) $2(\frac{1}{2},\frac{1}{2},0)$ $\ \ x,0,0$

(7) $2(\frac{1}{2},\frac{1}{2},0)$ $\ \ x,x,0$

(8) $2(\frac{1}{2},\frac{1}{2},0)$ $\ \ x,\bar{x},0$

(9) $\bar{1}$ $\quad \frac{1}{4},\frac{1}{4},0$

(10) $n(\frac{1}{2},\frac{1}{2},0)$ $\ \ x,y,0$

(11) $\bar{4}^+$ $\ \frac{1}{2},0,z; \ \frac{1}{2},0,0$

(12) $\bar{4}^-$ $\ \frac{1}{2},0,z; \ \frac{1}{2},0,0$

(13) m $\ \ x,0,z$

(14) m $\ \ 0,y,z$

(15) m $\ \ x,\bar{x},z$

(16) m $\ \ x,x,z$

Generators selected   (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
16 h 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk:\ h+k=2n$
	(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k:\ k=2n$
	(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h0:\ h=2n$
	(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	

Special: as above, plus

8 g $..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8 f $.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z$	$y,0,z$	no extra conditions
	$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$y+\frac{1}{2},\frac{1}{2},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}$	
8 e $..2$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
	$\bar{x}+\frac{1}{2},\bar{x},0$	$x+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	$\bar{x},x+\frac{1}{2},0$	
4 d $2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4 c $..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$hk:\ h,k=2n$
2 b $4mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2 a $\bar{4}m2$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I	[2] $p\bar{4}m2$ (59)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $p\bar{4}2_1m$ (58)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4mm$ (55)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p42_12$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $p4/n11$ ($p4/n$, 52)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $p2/n12/m$ ($cmme$, 48)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $p2/n2_1/m1$ ($pmmn$, 46)	1; 2; 5; 6; 9; 10; 13; 14

IIa   none

IIb   none

Maximal isotypic subgroups of lowest index

IIc   [9] $p4/nmm$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) (64)

Minimal non-isotypic supergroups

I   none

II   [2] $c4/mmm$ ($p4/mmm$, 61)

5.2. Guide to the use of the scanning tables

5.2.1. Introduction

The global symmetry of an ideal crystal is described by its space group $\mathcal{G}$. It is also of interest to consider symmetries of local character. The classical example is that of the site symmetries, which are the symmetries of individual points in a crystal. These are completely described and classified as a part of the standard description of space groups in *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 1983). The results of this procedure contain two types of information:

(i) site symmetries of individual points under the action of the group $\mathcal{G}$ and

(ii) orbits of points under the action of the group $\mathcal{G}$.

This information, apart from its use, for example, in the consideration of the splitting of atomic levels in the field of the site symmetry, provides the background for the description of crystal structure: points of the same orbit are occupied by identical atoms (ions) and the environment of these atoms (ions) is also identical. A complete description of the structure is reduced to a description of the occupation of individual Wyckoff positions.

Analogously, we may consider the symmetries of planes transecting the crystal and of straight lines penetrating the crystal, called here the *sectional layer groups* (*symmetries*) and the *penetration rod groups* (*symmetries*). Here we look again for the two types of information:

(i) symmetries of individual planes (straight lines) under the action of the group $\mathcal{G}$ and

(ii) orbits of planes (straight lines) under the action of the group $\mathcal{G}$.

The general law that describes the connection between local symmetries and orbits of points, planes or straight lines is expressed by a coset resolution of the space group with respect to local symmetries. The orbits of planes (straight lines) have analogous properties to orbits of points. The structure of the plane (straight line) and its environment is identical for different planes (straight lines) of the same orbit. This is useful in the consideration of layer structures, see Section 5.2.5.1, and of structures with pronounced rod arrangements.

Layer symmetries have also been found to be indispensable in *bicrystallography*, see Section 5.2.5.2. This term and the term *bicrystal* were introduced by Pond & Bollmann (1979) with reference to the study of grain boundaries [see also Pond & Vlachavas (1983) and Vlachavas (1985)]. A bicrystal is in general an edifice where two crystals, usually of the same structure but of different orientations, meet at a common boundary – an interface. The sectional layer groups are appropriate for both the description of symmetries of such boundary planes and the description of the bicrystals.

The *sectional layer groups* were, however, introduced much earlier by Holser (1958*a,b*) in connection with the consideration of domain walls and twin boundaries as symmetry groups of planes bisecting the crystal. The mutual orientations of the two components of a bicrystal are in general arbitrary. In the case of domain walls and twin boundaries, which can be considered as interfaces of special types of bicrystals, there are crystallographic restrictions on these orientations. The group-theoretical basis for an analysis of domain pairs is given by Janovec (1972). The consideration of the structure of domain walls or twin boundaries involves the sectional layer groups (Janovec, 1981; Zikmund,

1984); they were examined in the particular cases of domain structure in KSCN crystals (Janovec *et al.*, 1989) and of domain walls and antiphase boundaries in calomel crystals (Janovec & Zikmund, 1993), see Section 5.2.5.3, and recently also in fullerene C_{60} (Janovec & Kopský, 1997; Saint-Grégoire, Janovec & Kopský, 1997).

The first attempts to derive the sectional layer groups systematically were made by Wondratschek (1971) and by using a computer program written by Guigas (1971). Davies & Dirl (1993*a*) developed a program for finding subgroups of space groups, which they later modified to find sectional layer groups and penetration rod groups as well (Davies & Dirl, 1993*b*). The use and determination of sectional layer groups have also been discussed by Janovec *et al.* (1988), Kopský & Litvin (1989) and Fuksa *et al.* (1993).

The penetration rod groups can be used in the consideration of linear edifices in a crystal, *e.g.* line dislocations or intersections of boundaries, or in crystals with pronounced rod arrangements. So far, there seems to be no interest in the penetration rod groups and there is actually no need to produce special tables for these groups. Determining penetration rod groups was found to be a complementary problem to that of determining sectional layer groups (Kopský, 1989*c*, 1990).

The keyword for this part of this volume is the term *scanning*, introduced by Kopský (1990) for the description of the spatial distribution of local symmetries. In this sense, the description of site symmetries and classification of point orbits by Wyckoff positions are a result of the *scanning* of the space group for the site symmetries.

The *Scanning tables*, Part 6, give a complete set of information on the space distribution of sectional layer groups and of the penetration rod groups. They were derived using the *scanning-group* method and the *scanning theorem*, see Section 5.2.2.2. The tables describe explicitly the scanning for the sectional layer groups. The spatial distribution of (scanning for) the penetration rod groups is seen directly from the *scanning groups*, which are given as a part of the information in the scanning tables.

The sectional layer groups and the penetration rod groups are subgroups of space groups and as such act on the three-dimensional point space. The examples of particular studies in Section 5.2.5 emphasize the importance of the exact location of sectional layer groups with reference to the crystal structure and hence to the crystallographic coordinate system. In the usual interpretation, Hermann–Mauguin symbols do not specify the location of the group in space. In the scanning tables, each Hermann–Mauguin symbol means a quite specific space or layer group with reference to a specified crystallographic coordinate system, see Sections 5.2.3.1.1 and 5.2.3.1.4.

The layer and rod groups can also be interpreted as factor groups of reducible space groups (Kopský, 1986, 1988, 1989*a,b*, 1993*a*; Fuksa & Kopský, 1993). Our choice of standard Hermann–Mauguin symbols for frieze, rod and layer groups reflects the relationship between reducible space groups and subperiodic groups as their factor groups, see Section 1.2.17. In the case of the layer groups, our choice thus substantially differs from that made by Wood (1964). The interpretation of subperiodic groups as factor groups of reducible space groups also has consequences in the representation theory of space and subperiodic groups. Last but not least, this relationship reveals relations between the algebraic structure of the space group of a crystal and the
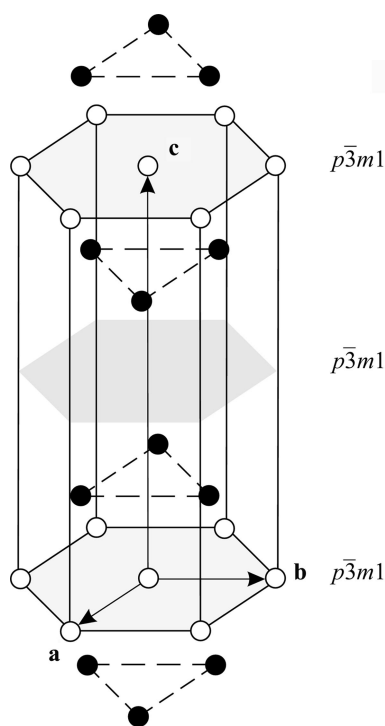
Fig. 5.2.5.1. The structure of cadmium iodide, CdI$_2$. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

horizontal lines in the tables of orientation orbits and auxiliary bases. The orbit contains six orientations in groups of the Laue class $m\bar{3}$ (T_h) and 12 orientations in groups of the Laue class $m\bar{3}m$ (O_h). The orbit turns into a special orbit with fixed parameters for the special values $m = 1$, $n = 0$ in groups of both the Laue classes $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h). The scanning changes from monoclinic/inclined to orthorhombic in the Laue class $m\bar{3}$ (T_h), to tetragonal in the Laue class $m\bar{3}m$ (O_h). The symmetry of the orientation also increases to orthorhombic for special values $m = 1$, $n = 1$ in groups of the Laue class $m\bar{3}m$ (O_h).

The choice of bases for the three subsets is the same as in orthorhombic groups, where the orientations of subsets are separated into three different orbits and the auxiliary bases are expressed in terms of vectors of the conventional cubic basis for the centring types P and I. For the centring type F, the Miller indices differ in the original and auxiliary basis. In this case, we express the Miller indices with reference to the original basis as $(hk0)$ and relate them to Miller indices $(mn0)$ with reference to the auxiliary bases. These relations are the same as in the case of F-centring in orthorhombic groups, see relations (5.2.4.2) and (5.2.4.3).

Orientation orbit (hhl): The orbit contains 12 orientations which divide into three subsets corresponding to the three main cubic axes. In each of the subsets, one of the vectors of the conventional cubic basis is chosen as the vector $\widehat{\mathbf{b}}$ of the auxiliary basis. The orientations of the subsets are separated by horizontal lines across the table. The first subset corresponds to the vector $\mathbf{c}$ of the cubic basis and the orientations in this subset are the same as in the (hhl) orbit for tetragonal groups of the Laue class $4/mmm$ (D_{4h}). The orientations within each subset are further divided into two pairs of orientations to which correspond two different unique axes of the monoclinic scanning group. These subsets are again separated by horizontal lines across the last two columns. For the centring types P and I and for the first subset of orientations, the description of orientations and bases coincides with the description of the orbit (hhl) in tetragonal groups of the Laue class $4/mmm$ (D_{4h}) and centring types P and I, including the choice of auxiliary and conventional bases of scanning groups and relations between Miller indices h, l and m, n. For the other

subsets of orientations, the data in tables are obtained by the cyclic permutation of vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$.

For the centring type F, orientation (hhl), we choose the auxiliary basis of the scanning group with the unique axis vectors $\widehat{\mathbf{c}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} + \mathbf{b})/2$, while for the orientation $(h\bar{h}l)$, we choose $\widehat{\mathbf{c}} = (\mathbf{a} + \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$. The bases for the remaining orientations are again obtained by the cyclic permutation of vectors of the conventional cubic basis.

Transformation of Miller indices: The straight line in which a plane (hhl) intersects with the plane $(1\bar{1}0)$ has the direction of a vector $(\mathbf{a} + \mathbf{b})/2h - \mathbf{c}/l$ or of the vector $\mathbf{b}' = n\widehat{\mathbf{a}} - m\mathbf{c} = n(\mathbf{a} + \mathbf{b})/2 - m\mathbf{c}$. As these two vectors can differ only by a numerical factor, the pair $(2m, n)$ must be proportional to the pair (h, l) and we obtain the relations

$$h \text{ odd } \Rightarrow m = h, n = 2l; \quad h \text{ even } \Rightarrow m = h/2, n = l,$$

recorded at the bottom row of the orientation-orbit table for the centring type F.

For the special values $h = 1$, $l = 0$, this orbit turns into an orbit (110) with fixed parameters and an orthorhombic scanning group.

5.2.5. Applications

5.2.5.1. *Layer symmetries in crystal structures*

The following two examples show the use of layer symmetries in the description of crystal structures.

Example 1: Fig. 5.2.5.1 shows the crystal structure of cadmium iodide, CdI$_2$. The space group of this crystal is $P\bar{3}m1$, D_{3d}^3 (No. 164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI$_2$ structure is:

A	C	B	C
I	Cd	I	void

From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

The plane at height $0\mathbf{c}$ contains cadmium ions. This plane defines the orbit of planes of orientation (0001) located at points $P + n\mathbf{c}$, where $n \in Z$ (Z is the set of all integers). All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $\frac{1}{2}\mathbf{c}$ defines the orbit of planes of orientation (0001) located at points $P + (n + \frac{1}{2})\mathbf{c}$, where $n \in Z$. All these planes lie midway between A and B layers of iodine ions with the B layer below, the A layer above the plane. They contain only voids.

The planes at levels $\frac{1}{4}\mathbf{c}$ and $\frac{3}{4}\mathbf{c}$ contain B and A layers of iodine ions, respectively. These planes and all planes produced by translations $n\mathbf{c}$ from them belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

Example 2: The space group of cadmium chloride, CdCl$_2$, is $R\bar{3}m$, D_{3d}^5 (No. 166). Fig. 5.2.5.2 shows the structure of CdCl$_2$ in its triple hexagonal cell. The anions form a cubic close packing of spheres and the cations occupy half of the octahedral holes of each alternate layer. In close-packing notation, the CdCl$_2$ structure is:

A	C	B	A	C	B	A	C	B	A	C	B
Cl	Cd	Cl	void	Cl	Cd	Cl	void	Cl	Cd	Cl	void

We choose the origin at a cadmium ion and the hexagonal basis vectors $\mathbf{a}$, $\mathbf{b}$ as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}$, $\frac{1}{6}\mathbf{c}$, $\frac{1}{3}\mathbf{c}$, $\frac{1}{2}\mathbf{c}$, $\frac{2}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ have a sectional layer group of the type $p\bar{3}m1$ (L72) and at any other height have a sectional layer group of the type $p3m1$ (L69).

No. 13 $P2/c$ C_{2h}^4

$$\mathcal{G} = P12/c1 \quad \text{UNIQUE AXIS } b$$

CELL CHOICE 1

$$\mathcal{G} = P112/a \quad \text{UNIQUE AXIS } c$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$			Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/a$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p112/a$	L07
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112\,(\mathbf{a}/4)$	L03
UNIQUE AXIS b ($n0m$)	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c ($mn0$)	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$P2/b11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2/b11$	L16
			q odd		$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12
			m odd	$P2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
			q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211\,(\mathbf{b}'/4)$	L08
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
			m odd	$P2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
		p odd	q even		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01

No. 13 $P2/c$ C_{2h}^4

$$\mathcal{G} = P12/n1 \quad \text{UNIQUE AXIS } b$$

CELL CHOICE 2

$$\mathcal{G} = P112/n \quad \text{UNIQUE AXIS } c$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$			Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
UNIQUE AXIS b (010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$P112/n$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p112/n$	L07
UNIQUE AXIS c (001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p112\,[(\mathbf{a}+\mathbf{b})/4]$	L03
UNIQUE AXIS b ($n0m$)	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$				
UNIQUE AXIS c ($mn0$)	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$				
		n odd	m even	$P2/n11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
		p even	q odd		$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211\,(\mathbf{b}'/4)$	L08
		or			$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
		n even	m odd				
		p odd	q even				
		p odd	q odd	$P2/c11$	$[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$	$p\bar{1}$	L02
					$[\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$	$p211$	L08
					$[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$	$p1$	L01
		n odd	m odd	$P2/b11$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p2/b11$	L16
					$[s\mathbf{d}, -s\mathbf{d}]$	$pb11$	L12

No. 224 $Pn\overline{3}m$ O_h^4

$$\mathcal{G} = P\tfrac{4_2}{n}\overline{3}\tfrac{2}{m} \quad \text{origin 2}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P4_2/nnm$	$[0\mathbf{d}, \tfrac{1}{2}\mathbf{d}]$	$\widehat{c}mme$	L48
(100)	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{a}$	(origin 2)	$[\tfrac{1}{4}\mathbf{d}, \tfrac{3}{4}\mathbf{d}]$	$p\overline{4}2m\,[(\mathbf{a}'+\mathbf{b}')/4]$	L57
(010)	$\mathbf{c}$	$\mathbf{a}$	$\mathbf{b}$	$(\mathbf{a}'/2 \text{ or } \mathbf{b}'/2)$	$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{2})\mathbf{d}]$	$\widehat{c}mm2\,[(\mathbf{a}'+\mathbf{b}')/4]$	L26
(110)	$\mathbf{c}$	$\mathbf{a}-\mathbf{b}$	$\mathbf{a}+\mathbf{b}$	$Abmm$	$[0\mathbf{d}, \tfrac{1}{2}\mathbf{d}]$	$pbmb$	L38
(011)	$\mathbf{a}$	$\mathbf{b}-\mathbf{c}$	$\mathbf{b}+\mathbf{c}$		$[\tfrac{1}{4}\mathbf{d}, \tfrac{3}{4}\mathbf{d}]$	$pbmm\,(\mathbf{b}'/4)$	L40
(101)	$\mathbf{b}$	$\mathbf{c}-\mathbf{a}$	$\mathbf{c}+\mathbf{a}$		$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{2})\mathbf{d}]$	$pbm2\,(\mathbf{b}'/4)$	L24
(1$\overline{1}$0)	$\mathbf{c}$	$\mathbf{a}+\mathbf{b}$	$\mathbf{b}-\mathbf{a}$	$Abmm$	$[0\mathbf{d}, \tfrac{1}{2}\mathbf{d}]$	$pbmm$	L40
(01$\overline{1}$)	$\mathbf{a}$	$\mathbf{b}+\mathbf{c}$	$\mathbf{c}-\mathbf{b}$	$[(\mathbf{b}'+\mathbf{d})/4]$	$[\tfrac{1}{4}\mathbf{d}, \tfrac{3}{4}\mathbf{d}]$	$pbmb\,(\mathbf{b}'/4)$	L38
($\overline{1}$01)	$\mathbf{b}$	$\mathbf{c}+\mathbf{a}$	$\mathbf{a}-\mathbf{c}$		$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{2})\mathbf{d}]$	$pbm2$	L24
(111)	$\mathbf{a}-\mathbf{b}$	$\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}$	With respect to origin at P			
($\overline{1}$11)	$\mathbf{b}-\mathbf{a}$	$-\mathbf{b}-\mathbf{c}$	$\boldsymbol{\tau}_3$	With respect to origin at $P+(\mathbf{a}+\mathbf{b})/2$			
(1$\overline{1}\overline{1}$)	$\mathbf{a}+\mathbf{b}$	$\mathbf{c}-\mathbf{b}$	$\boldsymbol{\tau}_1$	With respect to origin at $P+(\mathbf{b}+\mathbf{c})/2$			
($\overline{1}$1$\overline{1}$)	$-\mathbf{a}-\mathbf{b}$	$\mathbf{b}+\mathbf{c}$	$\boldsymbol{\tau}_2$	With respect to origin at $P+(\mathbf{c}+\mathbf{a})/2$			
				$R\overline{3}m$	$[0\mathbf{d}, \quad [\tfrac{1}{2}\mathbf{d},$	$p\overline{3}m1$	L72
					$\tfrac{1}{3}\mathbf{d}, \parallel \tfrac{5}{6}\mathbf{d},$	$p\overline{3}m1\,[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
					$\tfrac{2}{3}\mathbf{d}]\quad \tfrac{1}{6}\mathbf{d}]$	$p\overline{3}m1\,[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
					$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{3})\mathbf{d}, (\pm s+\tfrac{2}{3})\mathbf{d}]$	$p3m1$	L69

No. 225 $Fm\overline{3}m$ O_h^5

$$\mathcal{G} = F\tfrac{4}{n}\overline{3}\tfrac{2}{m}$$

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(001)	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\mathbf{c}$	$I4/mmm$	$[0\mathbf{d}, \tfrac{1}{2}\mathbf{d}]$	$p4/mmm$	L61
(100)	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$	$\mathbf{a}$		$[\tfrac{1}{4}\mathbf{d}, \tfrac{3}{4}\mathbf{d}]$	$p4/nmm$	L64
(010)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$	$\mathbf{b}$		$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{2})\mathbf{d}]$	$p4mm$	L55
(110)	$\mathbf{c}$	$(\mathbf{a}-\mathbf{b})/2$	$(\mathbf{a}+\mathbf{b})/2$	$Immm$	$[0\mathbf{d}, \tfrac{1}{2}\mathbf{d}]$	$pmmm$	L37
(1$\overline{1}$0)	$\mathbf{c}$	$(\mathbf{a}+\mathbf{b})/2$	$(\mathbf{b}-\mathbf{a})/2$		$[\tfrac{1}{4}\mathbf{d}, \tfrac{3}{4}\mathbf{d}]$	$pmmn\,[(\mathbf{a}'+\mathbf{b}')/4]$	L46
(011)	$\mathbf{a}$	$(\mathbf{b}-\mathbf{c})/2$	$(\mathbf{b}+\mathbf{c})/2$		$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{2})\mathbf{d}]$	$pmm2$	L23
(01$\overline{1}$)	$\mathbf{a}$	$(\mathbf{b}+\mathbf{c})/2$	$(\mathbf{c}-\mathbf{b})/2$				
(101)	$\mathbf{b}$	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{c}+\mathbf{a})/2$				
($\overline{1}$01)	$\mathbf{b}$	$(\mathbf{c}+\mathbf{a})/2$	$(\mathbf{a}-\mathbf{c})/2$				
(111)	$(\mathbf{a}-\mathbf{c})/2$	$(\mathbf{b}-\mathbf{a})/2$	$\boldsymbol{\tau}$	$R\overline{3}m$	$[0\mathbf{d}, \quad [\tfrac{1}{2}\mathbf{d},$	$p\overline{3}m1$	L72
($\overline{1}$11)	$(-\mathbf{a}-\mathbf{c})/2$	$(\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_3$		$\tfrac{1}{3}\mathbf{d}, \parallel \tfrac{5}{6}\mathbf{d},$	$p\overline{3}m1\,[(2\mathbf{a}'+\mathbf{b}')/3]$	L72
(1$\overline{1}\overline{1}$)	$(\mathbf{a}+\mathbf{c})/2$	$(-\mathbf{a}-\mathbf{b})/2$	$\boldsymbol{\tau}_1$		$\tfrac{2}{3}\mathbf{d}]\quad \tfrac{1}{6}\mathbf{d}]$	$p\overline{3}m1\,[(\mathbf{a}'+2\mathbf{b}')/3]$	L72
($\overline{1}$1$\overline{1}$)	$(\mathbf{c}-\mathbf{a})/2$	$(\mathbf{a}+\mathbf{b})/2$	$\boldsymbol{\tau}_2$		$[\pm s\mathbf{d}, (\pm s+\tfrac{1}{3})\mathbf{d}, (\pm s+\tfrac{2}{3})\mathbf{d}]$	$p3m1$	L69