

INTERNATIONAL TABLES  
FOR  
CRYSTALLOGRAPHY

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Brief Teaching Edition of  
*Volume A*  
SPACE-GROUP SYMMETRY

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*Edited by*  
THEO HAHN

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CONTENTS

No. 73	$Ibca$	126
No. 92	$P4_12_12$	128
No. 135	$P4_2/mbc$	130
No. 141	$I4_1/amd$ (origin choices 1 and 2)	132
No. 162	$P\bar{3}1m$	136
No. 164	$P\bar{3}m1$	138
No. 166	$R\bar{3}m$	140
No. 194	$P6_3/mmc$	144
No. 199	$I2_13$	146
No. 205	$Pa\bar{3}$	148
No. 225	$Fm\bar{3}m$	150
No. 227	$Fd\bar{3}m$ (origin choices 1 and 2)	154
Author index		162
Subject index		163

# Preface to the Fifth, Revised Edition

BY TH. HAHN

Volume A of *International Tables for Crystallography* was first published in 1983. Shortly after, in 1985, the *Brief Teaching Edition of Volume A* was prepared, of which the present volume is the Fifth Edition. It is based on the Fifth, Revised Edition of Volume A (2002).

The *Teaching Edition* consists of:

complete descriptions of the 17 plane groups, so useful for the teaching of symmetry;

24 selected space-group examples, of varying complexity and distributed over all seven crystal systems;

those basic text sections of Volume A which are necessary for the understanding and handling of space groups (Parts 1, 2, 3 and 5).

Note that space group No. 64 (*Cmce*) provides an example containing the 'double' glide plane *e*.

The purpose of the *Teaching Edition* is threefold:

(i) It should provide a handy (and inexpensive) tool for researchers and students to familiarize themselves with the use of the space-group tables in Volume A.

(ii) It is designed for use in classroom teaching, and with this aim in mind the price has been kept as low as possible. In order to achieve this, the material has been reprinted from Volume A without any changes, except for pagination; hence, this *Teaching Edition* contains references to sections which are only found in Volume A.

(iii) It may serve as a laboratory handbook because the 24 examples include most of the frequently occurring space groups, for both organic and inorganic crystals.

In addition to the 24 space groups given explicitly, further space groups may easily be derived by making use of the general-position entries for the maximal subgroups of types I (*translationengleich*) and IIa (*klassengleich decentred*) as described in Section 2.2.15.1: The numbers given refer to those coordinate triplets of the general position of the group which are retained in the maximal subgroup and thus characterize the subgroup completely. For those maximal subgroups which conventionally are referred to the same basis vectors and the same origin as the group, the 'standard description', as given in Volume A, is obtained.

This procedure is illustrated by the following example:

For space group No. 199,  $I2_13$  (p. 147), the following entries are given under

## Maximal non-isomorphic subgroups

I [3]  $I2_11$  ( $I2_12_12_1$ , 24) (1; 2; 3; 4)+

which has to be read as

$$(0, 0, 0) + \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) +$$

$$(1) x, y, z \quad (2) \bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$$

$$(3) \bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2} \quad (4) x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}.$$

This is identical with the general position of space group No. 24,  $I2_12_12_1$  (p. 217 of Volume A), which is a maximal *translationengleiche* subgroup of  $I2_13$  of index [3].

IIa [2]  $P2_13$  (198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

which has to be read as

$$(1) x, y, z \quad (2) \bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2} \quad \dots \quad (12) \bar{y} + \frac{1}{2}, \bar{z}, x + \frac{1}{2}.$$

This is identical with the general position of space group No. 198,  $P2_13$  (p. 611 of Volume A), which is a maximal *klassengleiche* (decentred) subgroup of  $I2_13$  of index [2].

(The other entries under I on p. 147 refer to four conjugate maximal *translationengleiche* subgroups of type  $R3$  and index [4]; these entries, however, are *not* based on the standard axes and origin of  $R3$ .)

Similar relations hold for the following examples:

$P\bar{1}$ (2)	yields	$P1$ (1)
$C12/m1$ (12)	yields	$C121$ (5); $C1m1$ (8); $P12/m1$ (10)
$C12/c1$ (15)	yields	$C1c1$ (9); $P12/c1$ (13); $P12_1/n1$ (14)
$Pmna$ (53)	yields	$P112_1/a$ (14); $P12/n1$ (13); $Pmn2_1$ (31)
$Cmce$ ( $Cmca$ ) (64)	yields	$Pbca$ (61)
$R\bar{3}m$ (166)	yields	$R32$ (155); $R\bar{3}$ (148); $R3m$ (160); $P\bar{3}m1$ (164)
$P6_3/mmc$ (194)	yields	$P6_322$ (182); $P6_3/m$ (176); $P6_3mc$ (186); $P\bar{3}m1$ (164); $P\bar{3}1c$ (163); $P62c$ (190)
$I2_13$ (199)	yields	$I2_12_12_1$ (24); $P2_13$ (198)
$Fm\bar{3}m$ (225)	yields	$Fm\bar{3}$ (202); $F432$ (209); $F43m$ (216); $Pm\bar{3}m$ (221); $Pn\bar{3}m$ (224)
$Fd\bar{3}m$ (227, origin 1)	yields	$Fd\bar{3}$ (203); $F4_132$ (210); $F43m$ (216).

It is an interesting exercise to complete this list for the 24 selected space groups and to extend it even to those maximal subgroups where the origin, the basis vectors, or both, are different from the group; in fact, to encourage this kind of 'playing' with space groups is one of the intentions of the *Teaching Edition*.

The Editor wishes to extend his sincere thanks to the International Union of Crystallography for making this inexpensive edition possible, to D. W. Penfold, M. H. Dacombe, S. E. Barnes and N. J. Ashcroft (Chester) for its technical preparation, and to a number of colleagues for counsel on the selection of material, especially D. W. J. Cruickshank (Manchester) and H. Wondratschek (Karlsruhe).

Aachen, November 2001

THEO HAHN

## SAMPLE PAGES

# 1.4. Graphical symbols for symmetry elements in one, two and three dimensions

BY TH. HAHN

## 1.4.1. Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Symmetry plane or symmetry line	Graphical symbol	Glide vector in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions) }		None	<i>m</i>
'Axial' glide plane Glide line (two dimensions) }		$\frac{1}{2}$ lattice vector along line in projection plane $\frac{1}{2}$ lattice vector along line in plane	<i>a, b or c</i> <i>g</i>
'Axial' glide plane		$\frac{1}{2}$ lattice vector normal to projection plane	<i>a, b or c</i>
'Double' glide plane* (in centred cells only)		Two glide vectors: $\frac{1}{2}$ along line parallel to projection plane, $\frac{1}{2}$ normal to projection plane	<i>e</i>
'Diagonal' glide plane		One glide vector with two components: $\frac{1}{2}$ along line parallel to projection plane, $\frac{1}{2}$ normal to projection plane	<i>n</i>
'Diamond' glide plane† (pair of planes; in centred cells only)		$\frac{1}{4}$ along line parallel to projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	<i>d</i>

\* For further explanations of the 'double' glide plane *e* see Note (iv) below and Note (x) in Chapter 1.3.

† See footnote § to Section 1.3.1.

## 1.4.2. Symmetry planes parallel to the plane of projection

Symmetry plane	Graphical symbol*	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Reflection plane, mirror plane		None	<i>m</i>
'Axial' glide plane		$\frac{1}{2}$ lattice vector in the direction of the arrow	<i>a, b or c</i>
'Double' glide plane† (in centred cells only)		Two glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	<i>e</i>
'Diagonal' glide plane		One glide vector with two components $\frac{1}{2}$ in the direction of the arrow	<i>n</i>
'Diamond' glide plane‡ (pair of planes; in centred cells only)		$\frac{1}{2}$ in the direction of the arrow; the glide vector is always half of a centring vector, i.e. one quarter of a diagonal of the conventional face-centred cell	<i>d</i>

\* The symbols are given at the upper left corner of the space-group diagrams. A fraction *h* attached to a symbol indicates two symmetry planes with 'heights' *h* and  $h + \frac{1}{2}$  above the plane of projection; e.g.  $\frac{1}{8}$  stands for  $h = \frac{1}{8}$  and  $\frac{5}{8}$ . No fraction means  $h = 0$  and  $\frac{1}{2}$  (cf. Section 2.2.6).

† For further explanations of the 'double' glide plane *e* see Note (iv) below and Note (x) in Chapter 1.3.

‡ See footnote § to Section 1.3.1.



## 2. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

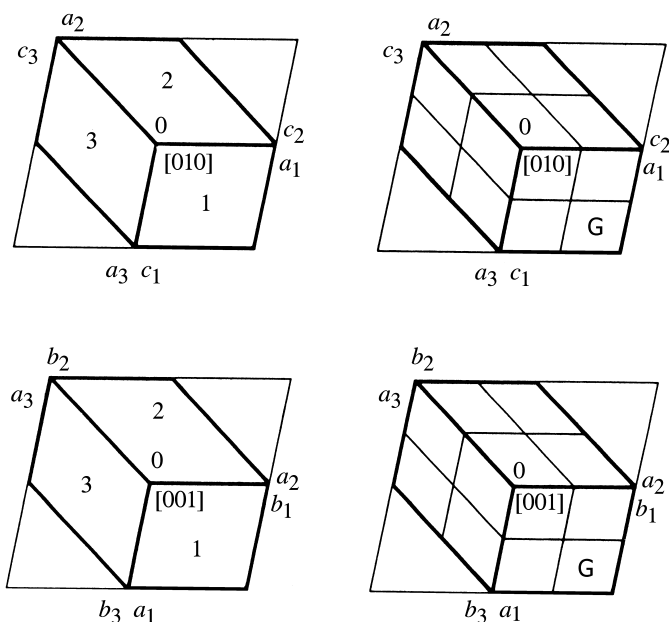


Fig. 2.2.6.4. Monoclinic space groups, cell choices 1, 2, 3. Upper diagrams: setting with unique axis  $b$ . Lower diagrams: setting with unique axis  $c$ . The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (cf. Section 2.2.16).

standard setting,  $\mathbf{a}, \mathbf{b}, \mathbf{c}$ , into those of the setting considered. For instance, the setting symbol  $\mathbf{cab}$  stands for the cyclic permutation

$$\mathbf{a}' = \mathbf{c}, \quad \mathbf{b}' = \mathbf{a}, \quad \mathbf{c}' = \mathbf{b}$$

or

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc}) \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{cab}),$$

where  $\mathbf{a}', \mathbf{b}', \mathbf{c}'$  is the new set of basis vectors. An interchange of two axes reverses the handedness of the coordinate system; in order to keep the system right-handed, each interchange is accompanied by the reversal of the sense of one axis, *i.e.* by an element  $\bar{1}$  in the transformation matrix. Thus,  $\mathbf{ba}\bar{c}$  denotes the transformation

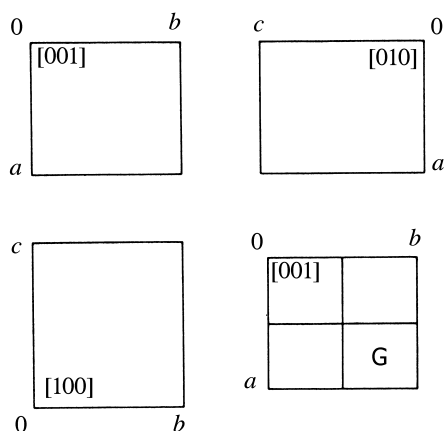


Fig. 2.2.6.5. Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc}) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} = (\mathbf{ba}\bar{c}).$$

The six orthorhombic settings correspond to six Hermann–Mauguin symbols which, however, need not all be different; cf. Table 2.2.6.1.\*

In the earlier (1935 and 1952) editions of *International Tables*, only one setting was illustrated, in a projection along  $c$ , so that it was usual to consider it as the 'standard setting' and to accept its cell edges as crystal axes and its space-group symbol as 'standard Hermann–Mauguin symbol'. In the present edition, however, *all six* orthorhombic settings are illustrated, as explained below.

The three projections of the symmetry elements can be interpreted in two ways. First, in the sense indicated above, that is, as different projections of a *single* (standard) setting of the space group, with the projected basis vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  labelled as in Fig. 2.2.6.5. Second, each one of the three diagrams can be considered as the projection along  $\mathbf{c}'$  of either one of *two different* settings: one setting in which  $\mathbf{b}'$  is horizontal and one in which  $\mathbf{b}'$  is vertical ( $\mathbf{a}', \mathbf{b}', \mathbf{c}'$  refer to the setting under consideration). This second interpretation is used to illustrate in the same figure the space-group symbols corresponding to these two settings. In order to view these projections in conventional orientation ( $\mathbf{b}'$  horizontal,  $\mathbf{a}'$  vertical, origin in the upper left corner, projection down the positive  $\mathbf{c}'$  axis), the setting with  $\mathbf{b}'$  horizontal can be inspected directly with the figure upright; hence, the corresponding space-group symbol is printed above the projection. The other setting with  $\mathbf{b}'$  vertical and  $\mathbf{a}'$  horizontal, however, requires turning the figure over  $90^\circ$ , or looking at it from the side; thus, the space-group symbol is printed at the left, and it runs upwards.

The 'setting symbols' for the six settings are attached to the three diagrams of Fig. 2.2.6.6, which correspond to those of Fig. 2.2.6.5. In the orientation of the diagram where the setting symbol is read in the usual way,  $\mathbf{a}'$  is vertical pointing downwards,  $\mathbf{b}'$  is horizontal pointing to the right, and  $\mathbf{c}'$  is pointing upwards from the page. Each setting symbol is printed in the position that in the space-group tables is actually occupied by the corresponding full Hermann–Mauguin symbol. The changes in the space-group symbol that are

\* A space-group symbol is invariant under sign changes of the axes; *i.e.* the same symbol applies to the right-handed coordinate systems  $\mathbf{abc}, \mathbf{a}\bar{\mathbf{b}}\bar{\mathbf{c}}, \bar{\mathbf{a}}\mathbf{b}\bar{\mathbf{c}}, \bar{\mathbf{a}}\bar{\mathbf{b}}\mathbf{c}$  and the left-handed systems  $\bar{\mathbf{a}}\bar{\mathbf{b}}\bar{\mathbf{c}}, \bar{\mathbf{a}}\mathbf{b}\mathbf{c}, \mathbf{a}\bar{\mathbf{b}}\mathbf{c}, \mathbf{a}\bar{\mathbf{b}}\bar{\mathbf{c}}$ .

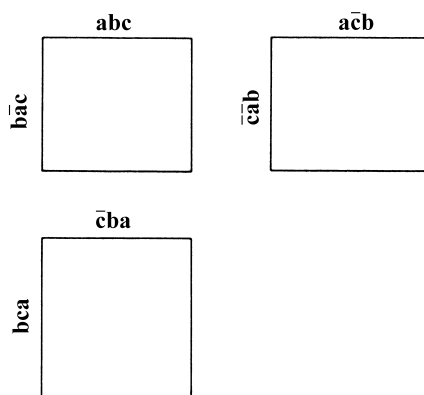


Fig. 2.2.6.6. Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by  $90^\circ$  or viewed from the side. Note that in the actual space-group tables instead of the setting symbols the corresponding full Hermann–Mauguin space-group symbols are printed.

$p6mm$

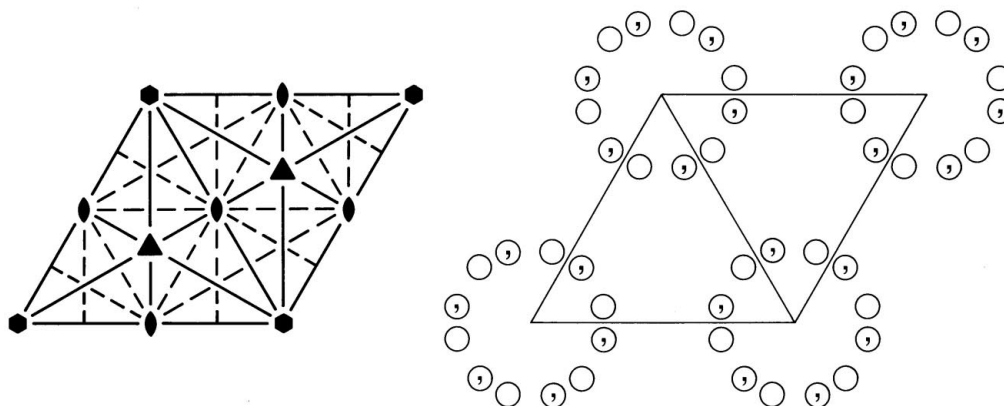
$6mm$

Hexagonal

No. 17

$p6mm$

Patterson symmetry  $p6mm$



Origin at  $6mm$

Asymmetric unit  $0 \leq x \leq \frac{2}{3}$ ;  $0 \leq y \leq \frac{1}{3}$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

Vertices  $0,0$   $\frac{1}{2},0$   $\frac{2}{3},\frac{1}{3}$

Symmetry operations

- |                     |                |                |
|---------------------|----------------|----------------|
| (1) 1               | (2) $3^+$ 0,0  | (3) $3^-$ 0,0  |
| (4) 2 0,0           | (5) $6^-$ 0,0  | (6) $6^+$ 0,0  |
| (7) $m$ $x,\bar{x}$ | (8) $m$ $x,2x$ | (9) $m$ $2x,x$ |
| (10) $m$ $x,x$      | (11) $m$ $x,0$ | (12) $m$ $0,y$ |

**Generators selected** (1);  $t(1,0)$ ;  $t(0,1)$ ; (2); (4); (7)

**Positions**

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

Reflection conditions

12	$f$	1	(1) $x, y$	(2) $\bar{y}, x-y$	(3) $\bar{x}+y, \bar{x}$
			(4) $\bar{x}, \bar{y}$	(5) $y, \bar{x}+y$	(6) $x-y, x$
			(7) $\bar{y}, \bar{x}$	(8) $\bar{x}+y, y$	(9) $x, x-y$
			(10) $y, x$	(11) $x-y, \bar{y}$	(12) $\bar{x}, \bar{x}+y$

General:

no conditions

Special: no extra conditions

6	$e$	$.m.$	$x, \bar{x}$	$x, 2x$	$2\bar{x}, \bar{x}$	$\bar{x}, x$	$\bar{x}, 2\bar{x}$	$2x, x$
6	$d$	$.m$	$x, 0$	$0, x$	$\bar{x}, \bar{x}$	$\bar{x}, 0$	$0, \bar{x}$	$x, x$
3	$c$	$2mm$	$\frac{1}{2}, 0$	$0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}$			
2	$b$	$3m.$	$\frac{1}{3}, \frac{2}{3}$	$\frac{2}{3}, \frac{1}{3}$				
1	$a$	$6mm$	$0, 0$					

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $p611$ ( $p6, 16$ )	1; 2; 3; 4; 5; 6
	[2] $p31m$ (15)	1; 2; 3; 10; 11; 12
	[2] $p3m1$ (14)	1; 2; 3; 7; 8; 9
	{ [3] $p2mm$ ( $c2mm, 9$ )	1; 4; 7; 10
	{ [3] $p2mm$ ( $c2mm, 9$ )	1; 4; 8; 11
	{ [3] $p2mm$ ( $c2mm, 9$ )	1; 4; 9; 12

**IIa** none**IIb** none**Maximal isomorphic subgroups of lowest index****IIc** [3]  $h6mm$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) ( $p6mm, 17$ )**Minimal non-isomorphic supergroups****I** none**II** none

$P2_1/c$

$C_{2h}^5$

$2/m$

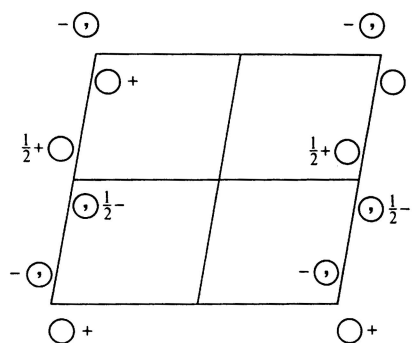
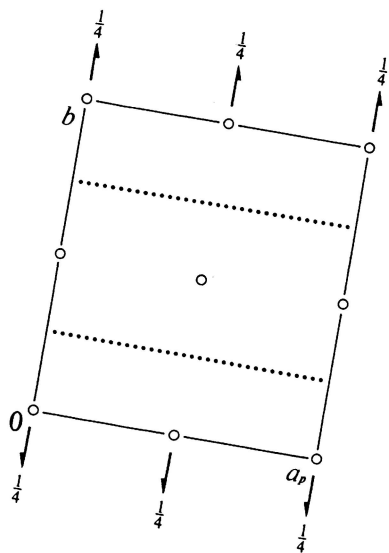
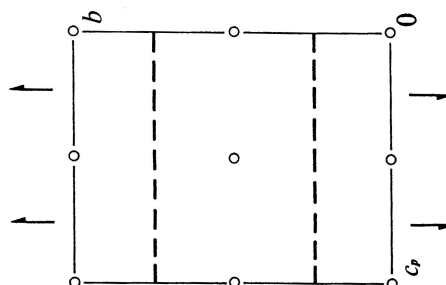
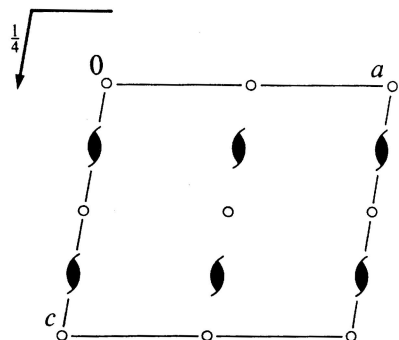
Monoclinic

No. 14

$P12_1/c1$

Patterson symmetry  $P12/m1$

UNIQUE AXIS  $b$ , CELL CHOICE 1



Origin at  $\bar{1}$

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

Symmetry operations

- (1) 1      (2)  $2(0, \frac{1}{2}, 0)$   $0, y, \frac{1}{4}$       (3)  $\bar{1}$   $0, 0, 0$       (4)  $c$   $x, \frac{1}{4}, z$

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
4 <i>e</i> 1	(1) $x, y, z$	(2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	General: $h0l : l = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : k + l = 2n$
2 <i>d</i> $\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : k + l = 2n$
2 <i>c</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$			$hkl : k + l = 2n$
2 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : k + l = 2n$
2 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl : k + l = 2n$

**Symmetry of special projections**

Along [001]  $p2gm$

$\mathbf{a}' = \mathbf{a}_p$      $\mathbf{b}' = \mathbf{b}$

Origin at 0, 0,  $z$

Along [100]  $p2gg$

$\mathbf{a}' = \mathbf{b}$      $\mathbf{b}' = \mathbf{c}_p$

Origin at  $x, 0, 0$

Along [010]  $p2$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$      $\mathbf{b}' = \mathbf{a}$

Origin at 0,  $y, 0$

**Maximal non-isomorphic subgroups**

**I**    [2]  $P1c1$  ( $Pc$ , 7)    1; 4  
       [2]  $P12_11$  ( $P2_1$ , 4)    1; 2  
       [2]  $P\bar{1}$  (2)    1; 3

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $P12_1/c1$  ( $\mathbf{a}' = 2\mathbf{a}$  or  $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$ ) ( $P2_1/c$ , 14); [3]  $P12_1/c1$  ( $\mathbf{b}' = 3\mathbf{b}$ ) ( $P2_1/c$ , 14)

**Minimal non-isomorphic supergroups**

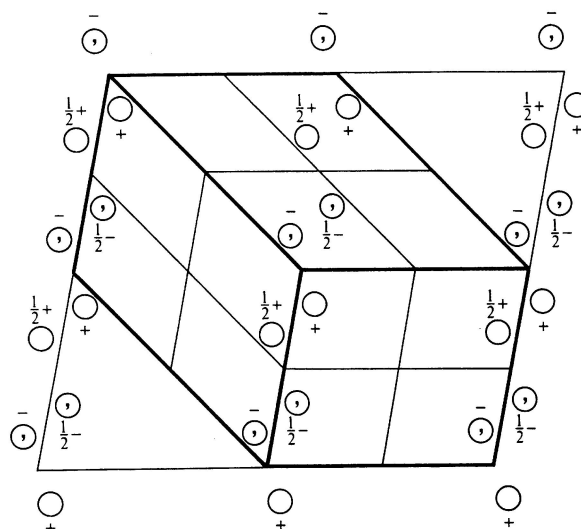
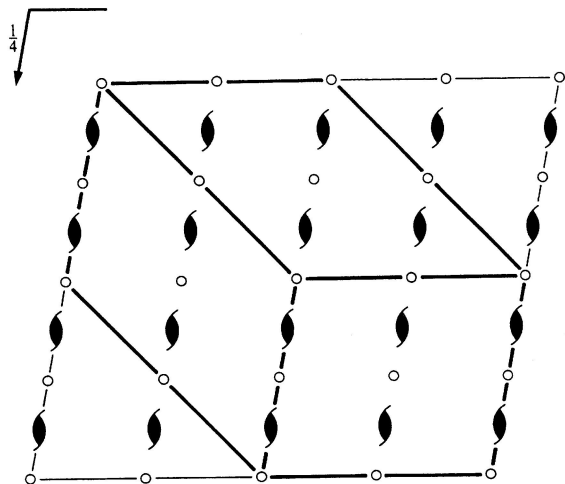
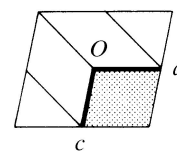
**I**    [2]  $Pnna$  (52); [2]  $Pmna$  (53); [2]  $Pcca$  (54); [2]  $Pbam$  (55); [2]  $Pccn$  (56); [2]  $Pbcm$  (57); [2]  $Pnrm$  (58); [2]  $Pbcn$  (60);  
       [2]  $Pbca$  (61); [2]  $Pnma$  (62); [2]  $Cmce$  (64)

**II**    [2]  $A12/m1$  ( $C2/m$ , 12); [2]  $C12/c1$  ( $C2/c$ , 15); [2]  $I12/c1$  ( $C2/c$ , 15); [2]  $P12_1/m1$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P2_1/m$ , 11);  
       [2]  $P12/c1$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $P2/c$ , 13)

$P2_1/c$  $C_{2h}^5$  $2/m$ 

Monoclinic

No. 14

UNIQUE AXIS  $b$ , DIFFERENT CELL CHOICES $P12_1/c1$ UNIQUE AXIS  $b$ , CELL CHOICE 1Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4	$e$	1	(1) $x, y, z$	(2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$
---	-----	---	---------------	---	---------------------------------	---

2	$d$	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
---	-----	-----------	-------------------------------	-------------------------------

2	$c$	$\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$
---	-----	-----------	---------------------	---------------------

2	$b$	$\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	---

2	$a$	$\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	-----------	-------------------------------

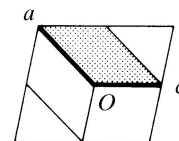
Reflection conditions

General:

 $h0l : l = 2n$  $0k0 : k = 2n$  $00l : l = 2n$ 

Special: as above, plus

 $hkl : k + l = 2n$  $hkl : k + l = 2n$  $hkl : k + l = 2n$  $hkl : k + l = 2n$

$P12_1/n1$ UNIQUE AXIS  $b$ , CELL CHOICE 2Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4	$e$	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$
---	-----	---	---------------	---	---------------------------------	---

Reflection conditions

General:

$h0l : h + l = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

$00l : l = 2n$

Special: as above, plus

$hkl : h + k + l = 2n$

$hkl : h + k + l = 2n$

$hkl : h + k + l = 2n$

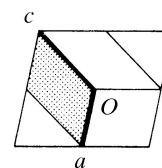
$hkl : h + k + l = 2n$

2	$d$	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	-------------------------------

2	$c$	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$
---	-----	-----------	-------------------------------	---------------------

2	$b$	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
---	-----	-----------	---------------------	-------------------------------

2	$a$	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	-----------	---

 $P12_1/a1$ UNIQUE AXIS  $b$ , CELL CHOICE 3Origin at  $\bar{1}$ Asymmetric unit  $0 \leq x \leq 1$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq 1$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4	$e$	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$
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Reflection conditions

General:

$h0l : h = 2n$

$0k0 : k = 2n$

$h00 : h = 2n$

Special: as above, plus

$hkl : h + k = 2n$

$hkl : h + k = 2n$

$hkl : h + k = 2n$

$hkl : h + k = 2n$

2	$d$	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	-----	-----------	---------------------	---

2	$c$	$\bar{1}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$
---	-----	-----------	---------------------	---------------------

2	$b$	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$
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2	$a$	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$
---	-----	-----------	-----------	-------------------------------