Réseau des Chercheurs et ITA Professionnels de la Cristallographie Structurale

ЯÉCIPROCS WORKSHOP

BILBAO CRYSTALLOGRAPHIC SERVER:

USEFUL DATABASES AND TOOLS IN PHASE-TRANSITION PROBLEMS

LECTURE BRIEFS

EXERCISES

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List of abbreviations

BC	Bradley, C. J. & Cracknell, A. P. (1972) The mathematical Theory of Symmetry in Solids. Oxford: Clarendon Press
BCS	The Bilbao Crystallographic Server (www.cryst.ehu.es)
BZ	Brillouin zone
CDML	Cracknell, A. P., Davies, B. L., Miller, S. C. & Love, W. F. (1979) Kronecker Product Tables. Vol. 1, General Introduction and Tables of Irreducible Representations of Space Groups. New York: IFI/Plenum
HM symbol	Hermann-Mauguin space-group symbol
*IT*A	International Tables for Crystallography, Vol. A (2016) Ed. Mois I. Aroyo. 6th ed. Chichester: John Wiley & Sons
irrep	irreducible representation
rep	representation

List of symbols

$\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{a}^*, \mathbf{k}$	vectors
x, y, z, k_x, k_y, k_z	point coordinates, vector coefficients
$\boldsymbol{x}, \boldsymbol{r}, \boldsymbol{w}$	column of point coordinates, of vector coefficients, of the translation part of a mapping
$\boldsymbol{A}, \boldsymbol{W}, \boldsymbol{I}$	$(n \times n)$ matrices
A_{ik}, B_{ik}, W_{ik}	matrix coefficients of matrices $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{W}$
$(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{W}, \boldsymbol{w})$	matrix–column pairs
$(\mathbf{a})^{\mathrm{T}}$	row of basis vectors
$\boldsymbol{A}^{\mathrm{T}}$	transposed matrix
$\mathrm{tr}(\boldsymbol{A})$	trace of the matrix $\boldsymbol{A}$
$\det(\boldsymbol{A})$	determinant of the matrix $\boldsymbol{A}$
$\mathbf{L}$	vector lattice
$\mathbf{k}$	vector of reciprocal space
$\star(\mathbf{k})$	star of vector $\mathbf{k}$
$\mathbf{K}$	vector of the reciprocal lattice [$\mathbf{h}$ in crystallographic literature]
$\mathbf{L}^*$	reciprocal lattice
$\mathbf{\Phi}$	representation domain
$\mathcal{G}$, $\mathcal{H}$, *422*	group, point group, space group
$\mathcal{T}$	tetrahedral group [same symbol as for the translation subgroup]
g, h, e, *1*, *2*	group elements

List of symbols, continued

D, $\mathsf{D}(\mathcal{G})$	rep, rep of group $\mathcal{G}$
$\mathsf{D}^{(i)}$	i-th irrep
$\chi(\mathsf{D})$	character of the rep D
$\chi(\mathsf{D}^{(i)})$	character of the irrep $\mathsf{D}^{(i)}$
$O(\mathsf{D}^{(i)}(\mathcal{H}))$	Orbit of the irrep $\mathsf{D}^{(i)}$ of $\mathcal{H} \lhd \mathcal{G}$
$\mathcal{G}^i \equiv \mathcal{G}^i(\mathsf{D}^{(i)}(\mathcal{H})),\ \mathcal{H} \lhd \mathcal{G}$	little group
$\boldsymbol{D}(g)$	matrix of the rep D, belonging to the group element g
$\boldsymbol{D}^{(i)}(g)$	matrix of the irrep $\mathsf{D}^{(i)}$, belonging to the group element g
$D^{(i)}(g)_{mn}$	m, n-th matrix element of the matrix $\boldsymbol{D}^{(i)}$ of irrep $\mathsf{D}^{(i)}$
$\dim(\mathsf{D}(\mathcal{G}))$	dimension of the rep D
$\mathsf{D}^{(i)} \otimes \mathsf{D}^{(j)}$	direct product of irreps $\mathsf{D}^{(i)}$ and $\mathsf{D}^{(j)}$
$\mathsf{D}^{(i)} \oplus \mathsf{D}^{(j)}$	direct sum of irreps $\mathsf{D}^{(i)}$ and $\mathsf{D}^{(j)}$
m_j or $m(\mathsf{D} \,\vert\, \mathsf{D}^{(j)})$	multiplicity of the j-th irrep in the rep D
$\mathsf{D}^{(i)}(\mathcal{G}) \downarrow \mathcal{H}$	rep of group $\mathcal{H}$ subduced from the irrep $\mathsf{D}^{(i)}(\mathcal{G})$
$\mathsf{D}^{(i)}(\mathcal{H}) \uparrow \mathcal{G}$	rep of group $\mathcal{G}$, induced from the irrep $\mathsf{D}^{(i)}(\mathcal{H})$
$(\mathsf{D}^{(i)}(\mathcal{H}))_g$	irrep $\mathsf{D}^{(i)}(\mathcal{H}), \mathcal{H} \lhd \mathcal{G}$, conjugated by the element $g \in \mathcal{G}$
$\mathcal{G}_0$	symmorphic space group
$\mathcal{T}$	translation subgroup of $\mathcal{G}$ [same symbol as for 'tetrahedral group']
$\overline{\mathcal{G}}$	point group of the space group $\mathcal{G}$
$\mathcal{G}^{\mathbf{k}}$	little group of vector $\mathbf{k}$ in space group $\mathcal{G}$
$\overline{\mathcal{G}}^{\mathbf{k}}$	little co-group of vector $\mathbf{k}$ in space group $\mathcal{G}$
$\mathbf{\Gamma}^{\mathbf{k}}$	irreps of the translation group $\mathcal{T}$
$\mathsf{D}^{\mathbf{k},i}$	i-th (allowed) irrep of the little group $\mathcal{G}^{\mathbf{k}}$
$\mathsf{D}^{(\star\mathbf{k}),i}$	i-th irrep of the space group $\mathcal{G}$, belonging to $\star\mathbf{k}$
$\overline{\mathsf{D}}^{\mathbf{k},i}$	i-th irrep of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$

Chapter 1

Symmetry data in *International Tables for Crystallography*, Volume A: Basic concepts and notation

1.1 Symmetry operations

1.1.1 Crystallographic Symmetry Operations and Their Representations by Matrices

In order to describe the symmetry operations analytically one introduces a coordinate system $\{O,\ \mathbf{a},\ \mathbf{b},\ \mathbf{c}\}$, consisting of a set of basis vectors $\mathbf{a},\ \mathbf{b},\ \mathbf{c}$ and an origin O. A symmetry operation can be regarded as an instruction of how to calculate the coordinates $\tilde{x}$, $\tilde{y}$, $\tilde{z}$ of the image point $\tilde{X}$ from the coordinates x, y, z of the original point X.
The equations are

$$\begin{aligned} \tilde{x} &= W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} &= W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} &= W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3, \end{aligned} \tag{1.1.1}$$

These equations can be written using the matrix formalism:

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} \qquad \text{where}$$

the symmetry operations $(\boldsymbol{W}, \boldsymbol{w})$ are given in a matrix-column form consisting of a (3×3) matrix (linear) part $\boldsymbol{W}$ and a (3×1)-column(translation) part $\boldsymbol{w}$:

$$(\boldsymbol{W},\ \boldsymbol{w}) = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \end{array}\right) \tag{1.1.2}$$

Apart from the matrix-column pair presentation of $(\boldsymbol{W}, \boldsymbol{w})$ often the so-called *short-hand notation* for the symmetry operations is used. It is obtained from the left-hand side of equ. (1.1.1) by omitting the terms with coefficients 0 and writing in one line the three different rows of equ.(1.1.1), separated by commas.

For example, consider the symmetry operation under No. 30 in the list of general positions obtained by the program `GENPOS` of the Bilbao Crystallographic Server (often referred to as BCS) for the space group $Pn\bar{3}n$, No. 222 (origin choice 2):

$\tilde{\boldsymbol{x}} = (\boldsymbol{W},\, \boldsymbol{w})\boldsymbol{x} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}$ would be

$\tilde{x} = 0\,x + 0\,y - 1\,z,\ \tilde{y} = 1\,x + 0\,y + 0\,z + 1/2,\ \tilde{z} = 0\,x + 1\,y + 0\,z + 1/2.$

The shorthand notation of $(\boldsymbol{W}, \boldsymbol{w})$ reads: $\overline{z}$, $x + 1/2$, $y + 1/2$.

1.1.2 Geometric Interpretation of the Matrix-column Pairs of Symmetry Operations

Geometric meaning of matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$

The geometric meaning of a matrix-column pair $(\boldsymbol{W}, \boldsymbol{w})$ can be determined only if the reference coordinate system is known. The following procedure indicates the necessary steps for the complete geometric characterization of $(\boldsymbol{W}, \boldsymbol{w})$.

Procedure for the geometric interpretation of $(\boldsymbol{W}, \boldsymbol{w})$

1. $\boldsymbol{W}$ -information

   (a) Type of isometry: the types 1,2,3,4,6 or $\bar{1}$,$\bar{2}$,$\bar{3}$,$\bar{4}$,$\bar{6}$ can be determined by the matrix invariants: $\det(\boldsymbol{W})$ and $\mathrm{tr}(\boldsymbol{W})$

	$\det(\boldsymbol{W}) = +1$					$\det(\boldsymbol{W}) = -1$				
$\mathrm{tr}(\boldsymbol{W})$	3	2	1	0	-1	-3	-2	-1	0	1
type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
order	1	6	4	3	2	2	6	4	6	2

   (b) Direction of $\boldsymbol{u}$ the rotation or rotoinversion axis or the normal of the reflection plane

      i. Rotations: Calculate the matrix $\boldsymbol{Y}(\boldsymbol{W}) = \boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I}$. The elements of any non-zero column of $\boldsymbol{Y}$ give the components of the vector $\boldsymbol{u}$ with respect to the reference co-ordinate system.

      ii. Rotoinversions: Calculate the matrix $\boldsymbol{Y}(-\boldsymbol{W})$. The elements of any non-zero column of $\boldsymbol{Y}$ give the components of the vector $\boldsymbol{u}$ with respect to the reference co-ordinate system. For $\bar{2} = m$, $\boldsymbol{Y}(-\boldsymbol{W}) = -\boldsymbol{W} + \boldsymbol{I}$.

   (c) Sense of rotation (for rotations or rotoinversions with $k > 2$): The sense of rotation is determined by the sign of the determinant of the matrix $\boldsymbol{Z}$, given by $\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\,\boldsymbol{W}\boldsymbol{x}]$, where $\boldsymbol{u}$ is the vector of 1b and $\boldsymbol{x}$ is a non-parallel vector of $\boldsymbol{u}$, *e.g.* one of the basis vectors.

2. $\boldsymbol{w}$ -information

   (a) Intrinsic translation part (screw or glide component) $\boldsymbol{t}$/k

      i. Screw rotations

$$\boldsymbol{t}/k = \frac{1}{k}\,\boldsymbol{Y}\,\boldsymbol{w}, \text{where}\, \boldsymbol{W}^k = \boldsymbol{I} \tag{1.1.3}$$

ii. Glide reflections

$$\boldsymbol{t}/k = \frac{1}{2}(\boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \tag{1.1.4}$$

(b) Location of the symmetry elements (fixed points $\boldsymbol{x}_F$)

i. $\boldsymbol{t}/k = 0$

$$(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}_F = \boldsymbol{x}_F. \tag{1.1.5}$$

ii. $\boldsymbol{t}/k \neq 0$

$$(\boldsymbol{W}, \boldsymbol{w}_{lp})\boldsymbol{x}_F = \boldsymbol{x}_F. \tag{1.1.6}$$

The column $\boldsymbol{w}_{lp} = \boldsymbol{w} - \boldsymbol{t}/k$ is the so-called *location part* as it determines the position of the rotation or screw-rotation axis or of the reflection or glide-reflection plane in space.

The formulæ of this section enable the user to find the geometric contents of any symmetry operation. In reality, *International Tables for Crystallography*, Vol. A (referred to as *IT*A in the following) provides the necessary information for all symmetry operations which are listed in the plane–group or space–group tables. The entries of the *General position* are numbered. The geometric meaning of these entries is listed under the same number in the block **Symmetry operations** in the tables of *IT*A. The explanation of the symbols for the symmetry operations is found in Sections 2.9 and 11.2 of *IT*A.

1.1.3 Symmetry Operations and Symmetry Elements

The definitions of *symmetry elements*, *geometric elements* and the related *element sets* of symmetry operations for crystallographic space groups and point groups are summarised in the following table.

Table 1.1.1 Symmetry elements in point and space groups

Name of symmetry element	Geometric element	Defining operation (d.o)	Operations in element set
Mirror plane	Plane A	Reflection in A	D.o. and its coplanar equivalents*
Glide plane	Plane A	Glide reflection in A; 2ν (not ν) a lattice translation	D.o. and its coplanar equivalents*
Rotation axis	Line b	Rotation around b, angle $2\pi/n$ $n = 2, 3, 4$ or 6	1st, ..., $(n-1)$th powers of d.o. and their coaxial equivalents†
Screw axis	Line b	Screw rotation around b, angle $2\pi/n$, $u = j/n$ times shortest lattice translation along b, right-hand screw, $n = 2, 3, 4$ or 6, $j = 1, \ldots, (n-1)$	1st, ..., $(n-1)$th powers of d.o. and their coaxial equivalents†
Rotoinversion axis	Line b and point P on b	Rotoinversion: rotation around b, angle $2\pi/n$, and inversion through P, $n = 3, 4$ or 6	D.o. and its inverse
Center	Point P	Inversion through P	D.o. only

* That is, all glide reflections with the same reflection plane, with glide vectors **v** differing from that of d.o. (taken to be zero for reflections) by a lattice translation vector. The glide planes a, b, c, d and e are distinguished.

† That is, all rotations and screw rotations with the same axis b, the same angle and sense of rotation and the same screw vector $\mathbf{u}$ (zero for rotation) up to a lattice translation vector.

1.2 Site symmetry: General and Special positions

The concept of *Site symmetry, i.e.* the set of symmetry operations that leave a given point fixed, allows to define *General* and *Special positions* for space groups.

Let $\mathcal{G}$ be a space group and X a point. The subgroup $\mathcal{S}_X = \{(\boldsymbol{W}, \boldsymbol{w})\}$ of all $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$ that leave X fixed, *i.e.* for which $(\boldsymbol{W}, \boldsymbol{w})X = X$ holds, is called the *site symmetry group* $\mathcal{S}_X$ of $\mathcal{G}$ for the point X. The group $\mathcal{S}_X < \mathcal{G}$ is of finite order. If $\mathcal{S}_X = \{I\}$, *i.e.* only the identity operation maps X onto itself, X is called a point of *General position*. Otherwise, if $\mathcal{S}_X > \{I\}$, X is called a point of *Special position*.

Each point X_i of a $\mathcal{G}$-orbit has its site symmetry group $\mathcal{S}_i < \mathcal{G}$. The site symmetry groups $\mathcal{S}_i$ and $\mathcal{S}_j$ of two points X_i and X_j of the same $\mathcal{G}$-orbit are conjugate subgroups of $\mathcal{G}$: if $X_j = (\boldsymbol{W}, \boldsymbol{w})X_i$, $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$, then $\mathcal{S}_j = (\boldsymbol{W}, \boldsymbol{w})\mathcal{S}_i(\boldsymbol{W}, \boldsymbol{w})^{-1}$. For this reason, all points of one special position in *IT*A are described by the same site-symmetry symbol.

In *IT*A the so-called *oriented site-symmetry symbols* are used to show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice. The oriented site-symmetry symbols of the site-symmetry groups display the same sequence of symmetry directions as the space-group symbol. Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot.

1.3 Coordinate Transformations: basic results

Let a coordinate system be given with a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ and an origin O. The general transformation (affine transformation) of the coordinate system consists of two parts, a linear part and a shift of the origin. The transformation is uniquely defined by the (3×3) matrix $\boldsymbol{P}$ of the linear part and the (3×1) column matrix $\boldsymbol{p}$ containing the components of the shift vector $\boldsymbol{p}$.

1. The linear part is described by a (3×3) matrix

$$\boldsymbol{P} = \begin{pmatrix} P_{11}\, P_{12}\, P_{13} \\ P_{21}\, P_{22}\, P_{23} \\ P_{31}\, P_{32}\, P_{33} \end{pmatrix}$$

   i.e. the matrix which relates the new basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)$ to the old basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ according to

$$(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3) = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)\ \boldsymbol{P} = (\mathbf{a}_1,\ \mathbf{a}_2, \mathbf{a}_3)\begin{pmatrix} P_{11}\, P_{12}\, P_{13} \\ P_{21}\, P_{22}\, P_{23} \\ P_{31}\, P_{32}\, P_{33} \end{pmatrix}. \tag{1.3.7}$$

2. A shift of the origin is defined by the *shift vector*

$$\boldsymbol{p} = (p_1\mathbf{a}_1, p_2\mathbf{a}_2, p_3\mathbf{a}_3)$$

   The basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are fixed at the origin O; the new basis vectors $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)$ are fixed at the new origin O' that has the coordinates (p_1, p_2, p_3) in the old coordinate system.

The general affine transformation of the coordinates of a point X in direct space (given by the column $\boldsymbol{x} = (x_1, x_2, x_3)$) is given by the following formula:

$$\boldsymbol{x}\,' = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x} = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p}). \tag{1.3.8}$$

The metric tensor $\boldsymbol{G}$ of the unit cell in direct lattice is transformed by the matrix $\boldsymbol{P}$ as follows:

$$\boldsymbol{G}\,' = \boldsymbol{P}^t\boldsymbol{G}\boldsymbol{P} \tag{1.3.9}$$

where $\boldsymbol{P}^t$ is the transposed matrix of $\boldsymbol{P}$.
The volume of the unit cell V changes with the transformation. The volume of the new unit cell V' is obtained by

$$V\,' = \det(\boldsymbol{P})V \tag{1.3.10}$$

with $\det(\boldsymbol{P})$ being the determinant of the matrix $\boldsymbol{P}$.
Also, the matrix-column pairs of the symmetry operations are changed by a change of the coordinate system. If a symmetry operation is described in the "old"(unprimed) coordinate system by the matrix-column pair ($\boldsymbol{W}$, $\boldsymbol{w}$) and in the "new"(primed) coordinate system by the pair ($\boldsymbol{W}\,'$, $\boldsymbol{w}\,'$), then the relation between the pairs ($\boldsymbol{W}$, $\boldsymbol{w}$) and ($\boldsymbol{W}\,'$, $\boldsymbol{w}\,'$) is given by:

$$(\boldsymbol{W}\,',\, \boldsymbol{w}\,') = (\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p}) \tag{1.3.11}$$

The coordinate systems of the space groups used by the programs and database on the Bilbao Crystallographic Server (referred to as *standard* or *default* settings) for the presentation of the space-group data coincide with the conventional space-group descriptions found in *IT*A. For space groups with more than one description in *IT*A, the following settings are chosen as standard: *unique axis b* setting, *cell choice* 1 for monoclinic groups, *hexagonal axes* setting for rhombohedral groups, and *origin choice 2* (origin in $\overline{1}$) for the centrosymmetric groups listed with respect to two origins in *IT*A. Optionally certain applications allow the usage of the so-called *IT*A settings which include all conventional settings applied in *IT*A (*e.g. rhombohedral axes* setting for rhombohedral groups, and *origin choice 1* for the centrosymmetric groups) and the great variety of about 530 settings of monoclinic and orthorhombic groups listed in Table 4.3.2.1 of *IT*A. Settings different from the standard ones and the *IT*A settings are designated as *non-conventional*.

1.4 Group-subgroup relations of space groups

1.4.1 Basic definitions

A subset $\mathcal{H}$ of elements of a group $\mathcal{G}$ is called a *subgroup* of $\mathcal{G}$, $\mathcal{G} > \mathcal{H}$ if it fulfills the group postulates with respect to the law of composition of $\mathcal{G}$. In general, the group $\mathcal{G}$ itself is included among the set of subgroups of $\mathcal{G}$, *i.e.* $\mathcal{G} \geq \mathcal{H}$. If $\mathcal{G} > \mathcal{H}$ is fulfilled, then the subgroup $\mathcal{H}$ is called a *proper* subgroup of $\mathcal{G}$. A subgroup $\mathcal{H} < \mathcal{G}$ is a *maximal subgroup* if no group $\mathcal{Z}$ exists for which $\mathcal{H} < \mathcal{Z} < \mathcal{G}$ holds.

Let $\mathcal{H} < \mathcal{G}$ be a subgroup of $\mathcal{G}$ of order $|\mathcal{H}|$. Because $\mathcal{H}$ is a proper subgroup of $\mathcal{G}$ there must be elements $g_q \in \mathcal{G}$ which are not elements of $\mathcal{H}$. Let $g_2 \in \mathcal{G}$ be one of them. Then the set of elements $g_2\,\mathcal{H} = \{g_2\,h_j \,|\, h_j \in \mathcal{H}\}$[1] is a subset of elements of $\mathcal{G}$ with the property that all its elements are different and that the sets $\mathcal{H}$ and $g_2\,\mathcal{H}$ have no element in common. Thus, also the set $g_2\,\mathcal{H}$ contains $|\mathcal{H}|$ elements of $\mathcal{G}$. If there is another element $g_3 \in \mathcal{G}$ which does belong neither to $\mathcal{H}$ nor to $g_2\,\mathcal{H}$, one can form another set $g_3\,\mathcal{H} = \{g_3\,h_j \,|\, h_j \in \mathcal{H}\}$. All elements of $g_3\,\mathcal{H}$ are different and no one occurs already in $\mathcal{H}$ or in $g_2\,\mathcal{H}$.

[1]The formulation $g_2\,\mathcal{H} = \{g_2\,h_j \,|\, h_j \in \mathcal{H}\}$ means: '$g_2\,\mathcal{H}$ is the set of the products $g_2\,h_j$ of g_2 with all elements $h_j \in \mathcal{H}$.'

This procedure can be continued until each element $g_r \in \mathcal{G}$ belongs to one of these sets. In this way the group $\mathcal{G}$ can be partitioned, such that each element $g \in \mathcal{G}$ belongs to exactly one of these sets.
The partition just described is called a *decomposition* $(\mathcal{G} : \mathcal{H})$ *into left cosets* of the group $\mathcal{G}$ relative to the group $\mathcal{H}$.

$$\mathcal{G} = \mathcal{H} \cup g_2\mathcal{H} \cup \cdots \cup g_i\mathcal{H} \tag{1.4.12}$$

The sets $g_p\,\mathcal{H},\ p = 1,\ \ldots,\ i$ are called *left cosets*, because the elements $h_j \in \mathcal{H}$ are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition into right cosets* $\mathcal{H}\,g_s$ if the elements $h_j \in \mathcal{H}$ are multiplied with the new elements g_s from the right-hand side.

$$\mathcal{G} = \mathcal{H} \cup \mathcal{H}g_2 \cup \cdots \cup \mathcal{H}g_i \tag{1.4.13}$$

The elements g_p or g_s are called the *coset representatives*. The number of cosets is called the *index* $[i] = |\mathcal{G} : \mathcal{H}|$ of $\mathcal{H}$ in $\mathcal{G}$.

Two subgroups $\mathcal{H}_j, \mathcal{H}_k < \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1}\mathcal{H}_j\,g_q = \mathcal{H}_k$ holds. In this way, the subgroups of $\mathcal{G}$ are distributed into classes of conjugate subgroups that are also called *conjugacy classes of subgroups*. Subgroups in the same conjugacy class are isomorphic and thus have the same order. Different conjugacy classes of subgroups may contain different numbers of subgroups, *i.e.* have different lengths.

A subgroup $\mathcal{H}$ of a group $\mathcal{G}$ is a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ if it is identical with all of its conjugates, $g_q^{-1}\mathcal{H}\,g_q = \mathcal{H}$, for all $g_q \in \mathcal{G}$, *i.e.* if its conjugacy class consists of the one subgroup $\mathcal{H}$ only.

1.4.2 Subgroups of space groups

The set of all symmetry operations of a three-dimensional crystal pattern forms its symmetry group, which is the *space group* of this crystal pattern. An essential feature of a crystal pattern is its periodicity which indicates that there are translations among its symmetry operations. The infinite number of translations determines the infinite order of any space group. The set of all translations of a space group $\mathcal{G}$ forms the infinite translation subgroup $\mathcal{T}(\mathcal{G}) \lhd \mathcal{G}$ which is a normal subgroup of $\mathcal{G}$ of finite index. Consider the right coset decomposition of $\mathcal{G}$ relative to $\mathcal{T}(\mathcal{G})$.

$$\begin{array}{lllll}
(\boldsymbol{I}, \boldsymbol{o}) & (\boldsymbol{W}_2,\ \boldsymbol{w}_2) & \ldots & (\boldsymbol{W}_m,\ \boldsymbol{w}_m) & \ldots & (\boldsymbol{W}_i,\ \boldsymbol{w}_i) \\
(\boldsymbol{I},\ \boldsymbol{t}_1) & (\boldsymbol{W}_2,\ \boldsymbol{w}_2 + \boldsymbol{t}_1) & \ldots & (\boldsymbol{W}_m,\ \boldsymbol{w}_m + \boldsymbol{t}_1) & \ldots & (\boldsymbol{W}_i,\ \boldsymbol{w}_i + \boldsymbol{t}_1) \\
(\boldsymbol{I},\ \boldsymbol{t}_2) & (\boldsymbol{W}_2,\ \boldsymbol{w}_2 + \boldsymbol{t}_2) & \ldots & (\boldsymbol{W}_m,\ \boldsymbol{w}_m + \boldsymbol{t}_2) & \ldots & (\boldsymbol{W}_i,\ \boldsymbol{w}_i + \boldsymbol{t}_2) \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
(\boldsymbol{I},\ \boldsymbol{t}_j) & (\boldsymbol{W}_2,\ \boldsymbol{w}_2 + \boldsymbol{t}_j) & \ldots & (\boldsymbol{W}_m,\ \boldsymbol{w}_m + \boldsymbol{t}_j) & \ldots & (\boldsymbol{W}_i,\ \boldsymbol{w}_i + \boldsymbol{t}_j) \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots
\end{array} .$$

Obviously, the coset representatives of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ represent in a clear and compact way the infinite number of elements of the space group $\mathcal{G}$. And this is one of the ways of presenting the space groups in ITA and also in the Bilbao Crystallographic Server, *i.e.* by the matrices of the coset representatives of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ listed in the *General position*.

Each coset in the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ is characterized by its linear part. One can show that the set of linear parts, represented by the set of matrices $\boldsymbol{W}_j$, forms a group which is called the *point group* $\mathcal{P}_\mathcal{G}$ of the space group $\mathcal{G}$. The point groups which can belong to space groups are called *crystallographic point groups*.
The following types of subgroups of space groups are to be distinguished:

A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is called a *translationengleiche subgroup* or a t-subgroup of $\mathcal{G}$ if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, *i.e.* $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$, *i.e.* the order of the point group $\mathcal{P}_\mathcal{G}$ is reduced.

A subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is called a *klassengleiche subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of $\mathcal{G}$ is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of $\mathcal{G}$ are retained. Then the number of cosets of the decompositions $(\mathcal{H} : \mathcal{T}(\mathcal{H}))$ and $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ is the same, *i.e.* the order of the point group $\mathcal{P}_\mathcal{H}$ is the same as that of $\mathcal{P}_\mathcal{G}$.

A *klassengleiche* or k-subgroup $\mathcal{H} < \mathcal{G}$ is called *isomorphic* or an *isomorphic subgroup* if it belongs to the same affine space-group type (isomorphism type) as $\mathcal{G}$ does.

A subgroup of a space group is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, *i.e.* point-group symmetry.

Subgroup specification Any subgroup $\mathcal{H}$ of a group $\mathcal{G}$ is related to a specific subset of elements of $\mathcal{G}$ and this subset defines the subgroup uniquely: different subgroups of $\mathcal{G}$, even those isomorphic to $\mathcal{H}$, correspond to different subsets of the elements of $\mathcal{G}$. For example, the listing of the maximal t-subgroups of the space groups in *IT*A is based on this fact: apart from the space-group type and index, each t-subgroup $\mathcal{H}$ is specified by the set of coordinate triplets of the general position of $\mathcal{G}$ which are retained in $\mathcal{H}$.

Any subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ can be specified by its *IT*A-number, the index in the group $\mathcal{G}$ and the transformation matrix-column pair $(\boldsymbol{P}, \boldsymbol{p})$ that relates the standard bases $(\mathbf{a}, \mathbf{b}, \mathbf{c})_\mathcal{H}$ of $\mathcal{H}$ and $(\mathbf{a}, \mathbf{b}, \mathbf{c})_\mathcal{G}$ of $\mathcal{G}$:

$$(\mathbf{a}, \mathbf{b}, \mathbf{c})_\mathcal{H} = (\mathbf{a}, \mathbf{b}, \mathbf{c})_\mathcal{G} \boldsymbol{P} \tag{1.4.14}$$

The column $\boldsymbol{p} = (p_1, p_2, p_3)$ of coordinates of the origin $O_\mathcal{H}$ of $\mathcal{H}$ is referred to the coordinate system of $\mathcal{G}$.
The subgroup data listed in the Bilbao Crystallographic Server, *i.e.* the space-group type of $\mathcal{H}$ and the transformation matrix $(\boldsymbol{P}, \boldsymbol{p})$, are completely sufficient to define the subgroup uniquely: the transformation of the coordinate triplets of general-position of $\mathcal{H}$ (in standard setting) to the coordinate system of $\mathcal{G}$ by $(\boldsymbol{P}, \boldsymbol{p})^{-1}$ yields exactly the subset of elements of $\mathcal{G}$ corresponding to $\mathcal{H}$.

Hermann theorem A very important result on group-subgroup relations between space groups is given by Hermann's theorem: For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group $\mathcal{M}$ with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where $\mathcal{M}$ is a *translationengleiche* subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{M}$. The decisive point is that any group-subgroup chain between space groups $\mathcal{G} > \mathcal{H}$ of index $[i]$ can be split into a *translationengleiche* subgroup chain between the space groups $\mathcal{G}$ and $\mathcal{M}$ of index $[i_P]$ and a *klassengleiche* subgroup chain between the space groups $\mathcal{M}$ and $\mathcal{H}$ of index $[i_L]$ where $[i] = [i_P] \cdot [i_L]$. The first one, also called t-chain $\mathcal{G} \overset{i_P}{>} \mathcal{M}$, is related to the reduction of the point-group symmetry in the subgroup. The second one $\mathcal{M} \overset{i_L}{>} \mathcal{H}_j$ is known also as k-chain and it takes account of the loss of translations.

It may happen, that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$. In other words, a maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup.

Maximal-subgroup chains If the maximal subgroups are known for each space group, then in principle each non-maximal subgroup of a space group $\mathcal{G}$ with finite index can be obtained from the data on

maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is connected with the original group $\mathcal{G}$ through a chain $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \cdots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where each group $\mathcal{Z}_j < \mathcal{Z}_{j-1}$ is a maximal subgroup of $\mathcal{Z}_{j-1}$, with the index $[i_j] = |\mathcal{Z}_{j-1} : \mathcal{Z}_j|$, $j = 1, \ldots, k$. The number k is finite and the relation $i = \prod_{j=1}^{k} i_j$ holds, *i.e.* the total index $[i]$ is the product of the indices i_j.

In a similar way, one can express the transformation matrix $(\boldsymbol{P}, \boldsymbol{p})$ for the symmetry reduction $\mathcal{G} \longrightarrow \mathcal{H}$ as a product of the transformation matrices $(\boldsymbol{P}, \boldsymbol{p})_j$ characterizing each of the intermediate steps $\mathcal{Z}_{j-1} > \mathcal{Z}_j$: $(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{P}, \boldsymbol{p})_1 (\boldsymbol{P}, \boldsymbol{p})_2 \cdots (\boldsymbol{P}, \boldsymbol{p})_k$ (here the matrices $(\boldsymbol{P}, \boldsymbol{p})_j$ relate the bases of $\mathcal{Z}_{j-1}$ and $\mathcal{Z}_j$, *i.e.* $(\mathbf{a}, \mathbf{b}, \mathbf{c})_j = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{j-1} \boldsymbol{P}_j$).

1.4.3 Minimal supergroups

In the previous sections the relation $\mathcal{H} < \mathcal{G}$ has been seen from the viewpoint of the group $\mathcal{G}$. In this case $\mathcal{H}$ was a subgroup of $\mathcal{G}$. However, the same relation may be viewed from the group $\mathcal{H}$. In that case $\mathcal{G} > \mathcal{H}$ is a *supergroup* of $\mathcal{H}$. As for the subgroups of $\mathcal{G}$, different kinds of supergroups of $\mathcal{H}$ may be distinguished. The following definitions are obvious:

Let $\mathcal{H} < \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$. Then $\mathcal{G} > \mathcal{H}$ is called a *minimal supergroup* of $\mathcal{H}$.

If $\mathcal{H}$ is a *translationengleiche* subgroup of $\mathcal{G}$ then $\mathcal{G}$ is a *translationengleiche supergroup* (*t-supergroup*) of $\mathcal{H}$.

If $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *klassengleiche supergroup* (*k-supergroup*) of $\mathcal{H}$.

If $\mathcal{H}$ is an isomorphic subgroup of $\mathcal{G}$, then $\mathcal{G}$ is an *isomorphic supergroup* of $\mathcal{H}$.

If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *general supergroup* of $\mathcal{H}$.

Following from Hermann's Theorem, a minimal supergroup of a space group is either a *translationengleiche* supergroup (*t*-supergroup) or a *klassengleiche* supergroup (*k*-supergroup). A proper minimal *t*-supergroup has always an index i, $1 < i < 5$, and is never isomorphic. A minimal *k*-supergroup with index i, $1 < i < 5$, may be isomorphic or non-isomorphic; for indices $i > 4$ a minimal *k*-supergroup can only be an isomorphic *k*-supergroup. The propositions, theorems and their corollaries of for maximal subgroups are valid correspondingly for minimal supergroups.

Subgroups of space groups of finite index are always space groups again. This does not hold for supergroups. For example, the direct product $\mathcal{G}$ of a space group $\mathcal{H}$ with a group of order 2 is not a space group although $\mathcal{H} < \mathcal{G}$ is a subgroup of index 2 of $\mathcal{G}$. Moreover, supergroups of space groups may be affine groups which are only isomorphic to space groups but not space groups themselves.

In the following we restrict the considerations to supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ which are themselves space groups. This holds, for example, for the symmetry relations between crystal structures when the symmetries of both structures can be described by space groups. Quasicrystals, incommensurate phases *etc.* are thus excluded. Even under this restriction, supergroups show a much more variable behaviour than subgroups do.

In general, the search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this difficulty is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group $\mathcal{G}$ itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group $\mathcal{E}$ of all isometries. For example, there is only a finite number of subgroups $\mathcal{H}$ of any space group $\mathcal{G}$ for any given index i. On the other hand, there may be not only an infinite number of supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ for a finite index i but even an uncountably infinite number of supergroups of $\mathcal{H}$. As an example, consider the group $\mathcal{H} = P1$. Then there is an infinite number of *t*-supergroups $P\overline{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\overline{1}$.

It is important to note that the t supergroups represent space groups only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. This requirement is always satisfied if the group $\mathcal{H}$ and the supergroup $\mathcal{G}$ belong to the same crystal family. If $\mathcal{G}$ is a k-supergroup of $\mathcal{H}$, $\mathcal{G}$ and $\mathcal{H}$ always belong to the same crystal family, and there are no lattice restrictions on $\mathcal{H}$. In that sense the lattice conditions are useful in the search for supergroups $\mathcal{G} > \mathcal{H}$ which are space groups, *i. e.* form the symmetry of crystal structures. Whereas a subgroup $\mathcal{H} < \mathcal{G}$ does not become noticeable in the lattice parameters of a space group $\mathcal{G}$, a space group $\mathcal{G} > \mathcal{H}$ of another crystal family must be indicated by the lattice parameters of the space group $\mathcal{H}$. Thus it may be an important advantage if the conditions of temperature, pressure or composition allow to start the search for possible phase transitions at the low-symmetry phase.

1.5 Generation of Crystallographic Groups

1.5.1 Crystallographic point-groups and abstract groups

In this section we describe shortly the relation of the point groups to their abstract groups. There are four kinds of abstract groups:

- Cyclic groups
- Abelian non-cyclic groups
- non-Abelian groups
- direct products of non-Abelian groups with the cyclic group of order 2.

The types of crystallographic point groups, *i. e.* the crystal classes, are distinguished by the geometric meaning of their groups of symmetry operations of the macroscopic crystals. In algebraic terms, the classification principle is the *affine equivalence* of matrix groups, *cf.* IT A, Section 8.2.3. In this respect, an inversion, a two-fold rotation, and a reflection are clearly to be distinguished. However, considered as groups together with the identity operation, these three symmetries belong to the same type of groups, also called the same *abstract group*, which is here "$\mathcal{C}_2$, the cyclic group of order 2". Isomorphic point groups may belong to different crystal classes but point groups of the same crystal class belong always to the same abstract group, *i. e.* are isomorphic.

The representations of the groups are properties of the abstract groups. Therefore, isomorphic point groups, *i. e.* point groups belonging to the same abstract group, have the same irreps. Instead of the 32 types of point groups or crystal classes, only 18 different abstract groups have to be distinguished. In Table 1.5.1 the classification of the 32 crystal classes into 18 abstract groups is displayed. In order to be able to distinguish the symbols for crystallographic point groups from those of the abstract groups, the crystallographic point groups are designated by their HM symbols; the corresponding abstract groups by Schoenflies symbols. These symbols are assumed to be known; they can be found in IT A or in any textbook of crystallography.

The derivation of the 32 crystal classes can be found in many textbooks, either by geometric, *e. g.* Buerger (1956), or by a mixture of geometric and algebraic arguments, *e. g.* Burckhardt (1966), Rigault (1980). The crystal classes and their irreducible representations (irreps) can be easily determined once the 18 abstract groups and their irreps are known.

Table 1.5.1 The crystallographic point groups as abstract groups

Symbol	order	HM symbols
$\mathcal{C}_1$	1	1
$\mathcal{C}_2$	2	2, m, $\overline{1}$
$\mathcal{C}_3$	3	3
$\mathcal{C}_4$	4	4, $\overline{4}$
$\mathcal{C}_6 \equiv \mathcal{C}_3 \times \mathcal{C}_2$	6	$\overline{3}$, 6, $\overline{6}$
$\mathcal{D}_2 \equiv \mathcal{C}_2 \times \mathcal{C}_2$	4	$2/m$, 222, $mm2$
$\mathcal{D}_3$	6	32, $3m$
$\mathcal{D}_4$	8	422, $4mm$, $\overline{4}2m$
$\mathcal{D}_6 \equiv \mathcal{D}_3 \times \mathcal{C}_2$	12	$\overline{3}m$, 622, $6mm$, $\overline{6}2m$
$\mathcal{D}_{2h} \equiv \mathcal{C}_2 \times \mathcal{C}_2 \times \mathcal{C}_2$	8	mmm
$\mathcal{C}_{4h} \equiv \mathcal{C}_4 \times \mathcal{C}_2$	8	$4/m$
$\mathcal{C}_{6h} \equiv \mathcal{C}_6 \times \mathcal{C}_2$	12	$6/m$
$\mathcal{D}_{4h} \equiv \mathcal{D}_4 \times \mathcal{C}_2$	16	$4/mmm$
$\mathcal{D}_{6h} \equiv \mathcal{D}_6 \times \mathcal{C}_2$	24	$6/mmm$
$\mathcal{T}$	12	23
$\mathcal{T}_h \equiv \mathcal{T} \times \mathcal{C}_2$	24	$m\overline{3}$
$\mathcal{O}$	24	432, $\overline{4}3m$
$\mathcal{O}_h \equiv \mathcal{O} \times \mathcal{C}_2$	48	$m\overline{3}m$

First column: Schoenflies symbol for the abstract group: $\mathcal{C}$ cyclic group; $\mathcal{D}$ dihedral group; $\mathcal{T}$ tetrahedral group; $\mathcal{O}$ octahedral group. '$\times$' means 'direct product'
Second column: group order
Third column: short Hermann-Mauguin symbols of the crystallographic point groups

1.5.2 Solvable Groups

Abelian groups and the remaining groups $\mathcal{D}_3$, $\mathcal{D}_4$, $\mathcal{T}$, and $\mathcal{O}$, *i. e.* all abstract groups of crystallographic point groups are solvable groups.
Definition (D 1.5.2.1) A group $\mathcal{G}$ is called a *solvable group* or a *soluble group* if a series of subgroups $\mathcal{H}_i$ exists

$$\mathcal{G} \rhd \mathcal{H}_1 \rhd \cdots \rhd \mathcal{H}_{n-1} \rhd \mathcal{H}_n = \mathcal{I},$$

such that the factor groups $\mathcal{H}_i/\mathcal{H}_{i+1}$ of the pairs $\mathcal{H}_1 \lhd \mathcal{G}, \mathcal{H}_2 \lhd \mathcal{H}_1$, *etc.* are cyclic groups of prime order.

In this series which is called a *composition series* each of the subgroups $\mathcal{H}_i$ is a normal subgroup of the group $\mathcal{H}_{i-1}$ but not necessarily of the groups $\mathcal{H}_k$ with $k < i-1$. In particular, $\mathcal{H}_i$, $i > 1$, need not be a normal subgroup of $\mathcal{G}$. The group $\mathcal{I}$ (*identity group*) is the group consisting of the unit element $\boldsymbol{e}$ only.

1.5.3 Generation of Point Groups

A set of generators of a group is a subset of the group elements which by proper combination permits the generation of all elements of the group. Different sets of generators are possible. In *IT*A the generation

of the point groups by composition series is used. It is displayed in Figs. 1.5.1 and 1.5.2. A solid line connects a pair group – normal subgroup; a horizontal dashed arrow to the left points from the subgroup to the direct product with $\bar{1}$. The symbols at the solid lines are those of the generators which generate the group from the normal subgroup. Because of its importance for the derivation of the irreps, this kind of generation is also described in Tables 1.5.2 and 1.5.3.

Important for the calculation of the irreps in the next chapter is the observation that all factor groups in these series have orders 2 or 3, *i. e.* are cyclic groups of orders 2 and 3.

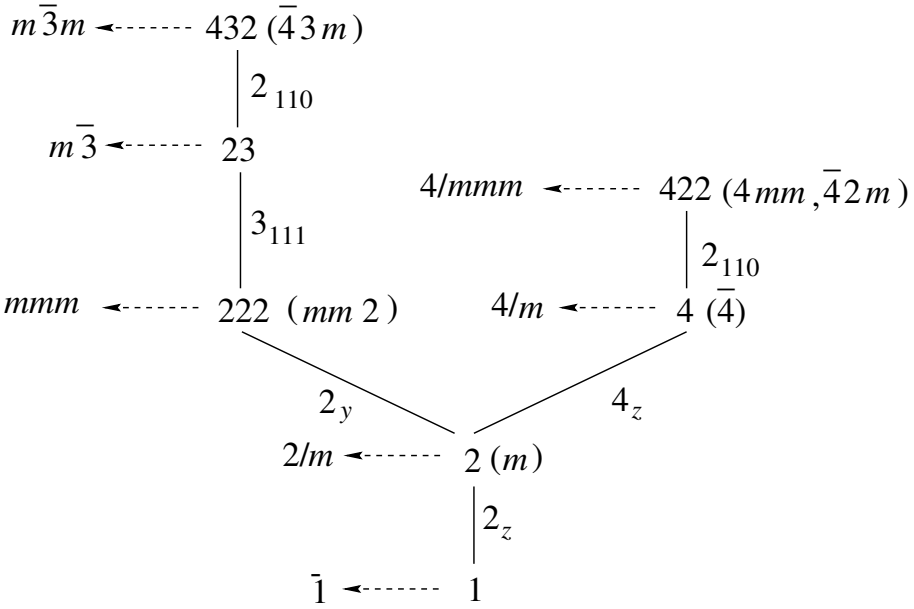


Fig. 1.5.1 Generation of sub-cubic point groups, see Tab. 1.5.2

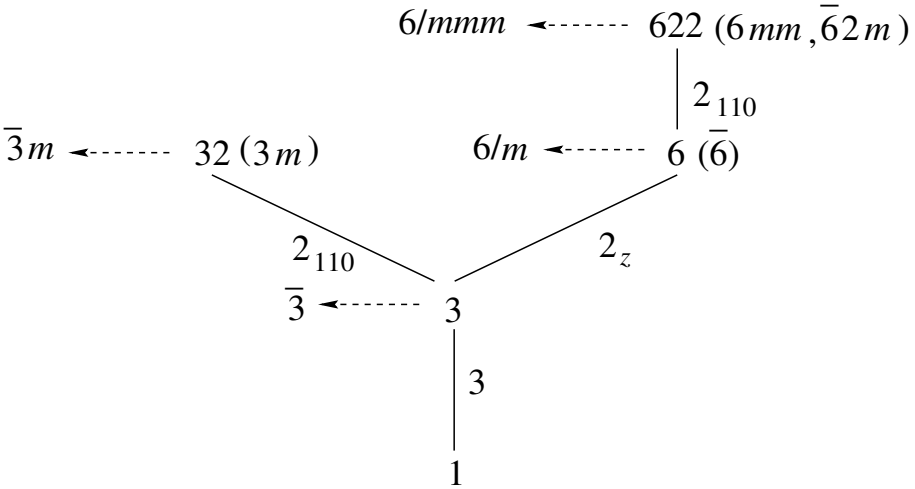


Fig. 1.5.2 Generation of sub-hexagonal point groups, see Tab. 1.5.3

Table 1.5.2 The generation of sub-cubic point groups

HM Symbol	SchoeSy	generators	compos. series
1	$\mathcal{C}_1$	1	1
$\overline{1}$	$\mathcal{C}_i$	1, $\overline{1}$	$\overline{1} \rhd 1$
2	$\mathcal{C}_2$	1, 2	$2 \rhd 1$
m	$\mathcal{C}_s$	1, m	$m \rhd 1$
$2/m$	$\mathcal{C}_{2h}$	1, 2, $\overline{1}$	$2/m \rhd 2 \rhd 1$
222	$\mathcal{D}_2$	1, 2_z, 2_y	$222 \rhd 2 \rhd 1$
$mm2$	$\mathcal{C}_{2v}$	1, 2_z, m_y	$mm2 \rhd 2 \rhd 1$
mmm	$\mathcal{D}_{2h}$	1, 2_z, 2_y, $\overline{1}$	$mmm \rhd 222 \rhd \ldots$
4	$\mathcal{C}_4$	1, 2_z, 4	$4 \rhd 2 \rhd 1$
$\overline{4}$	$\mathcal{S}_4$	1, 2_z, $\overline{4}$	$\overline{4} \rhd 2 \rhd 1$
$4/m$	$\mathcal{C}_{4h}$	1, 2_z, 4, $\overline{1}$	$4/m \rhd 4 \rhd \ldots$
422	$\mathcal{D}_4$	1, 2_z, 4, 2_y	$422 \rhd 4 \rhd \ldots$
$4mm$	$\mathcal{C}_{4v}$	1, 2_z, 4, m_y	$4mm \rhd 4 \rhd \ldots$
$\overline{4}2m$	$\mathcal{D}_{2d}$	1, 2_z, $\overline{4}$, 2_y	$\overline{4}2m \rhd \overline{4} \rhd \ldots$
$4/mmm$	$\mathcal{D}_{4h}$	1, 2_z, 4, 2_y, $\overline{1}$	$4/mmm \rhd 422 \rhd \ldots$
23	$\mathcal{T}$	1, 2_z, 2_y, 3_{111}	$23 \rhd 222 \rhd \ldots$
$m\overline{3}$	$\mathcal{T}_h$	1, 2_z, 2_y, 3_{111},$\overline{1}$	$m\overline{3} \rhd 23 \rhd \ldots$
432	$\mathcal{O}$	1, 2_z, 2_y, 3_{111}, 2_{110}	$432 \rhd 23 \rhd \ldots$
$\overline{4}3m$	$\mathcal{T}_d$	1, 2_z, 2_y, 3_{111}, $m_{1\overline{1}0}$	$\overline{4}3m \rhd 23 \rhd \ldots$
$m\overline{3}m$	$\mathcal{O}_h$	1, 2_z, 2_y, 3_{111}, 2_{110}, $\overline{1}$	$m\overline{3}m \rhd 432 \rhd \ldots$

Composition series of point group $m\overline{3}m$ and its subgroups, see also Fig. 1.5.1. For the longer composition series only the first members are listed.

1.5.4 Generation of Space Groups

In *IT*A the generators and the generating procedure of the space groups have been chosen such as to make the entries in the blocks of *General position* and *Symmetry operations* as transparent as possible. Given the set of h generators $\mathsf{G}_1, \mathsf{G}_2, \ldots, \mathsf{G}_p, \ldots \mathsf{G}_h$, any space-group operation W is generated by the following algorithm, starting with the identity and the translations as right-most factors:

$$\mathsf{W} = \mathsf{G}_h^{k_h}.\mathsf{G}_{h-1}^{k_{h-1}}.\ldots.\mathsf{G}_p^{k_p}.\ldots.\mathsf{G}_3^{k_3}.\mathsf{G}_2^{k_2}.\mathsf{G}_1. \tag{1.5.15}$$

Here, the exponents k_p are positive or negative integers, including zero.
The space-group generator G_1 is the identity (zero translation). It is chosen first and assures that the general position of $\mathcal{G}$ starts with the coordinate triplet x, y, z.The following generatorsG_2, G_3, G_4 are the translations corresponding to the three basis vectors **a**, **b**, **c** and G_5, G_6 are the generators for the centring translations, if present. The rest of the generators G_7, G_8, ... give all those symmetry operations of the space group $\mathcal{G}$ which are not pure translations. They have been chosen such that their exponents can assume only the values 0,1 and 2. Space groups of the same crystal class are generated in the same

Table 1.5.3 The generation of sub-hexagonal point groups

HM Symbol	SchoeSy	generators	compos. series
1	$\mathcal{C}_1$	1	1
3	$\mathcal{C}_3$	1, 3	$3 \rhd 1$
$\overline{3}$	$\mathcal{S}_6$	1, 3, $\overline{1}$	$\overline{3} \rhd 3 \rhd 1$
32	$\mathcal{D}_3$	1, 3, 2_{110}	$32 \rhd 3 \rhd 1$
$3m$	$\mathcal{C}_{3v}$	1, 3, m_{110}	$3m \rhd 3 \rhd 1$
$\overline{3}m$	$\mathcal{D}_{3d}$	1, 3, 2_{110}, $\overline{1}$	$\overline{3}m \rhd 32 \rhd \ldots$
6	$\mathcal{C}_6$	1, 3, 2_z	$6 \rhd 3 \rhd 1$
$\overline{6}$	$\mathcal{C}_{3h}$	1, 3, m_z	$\overline{6} \rhd 3 \rhd 1$
$6/m$	$\mathcal{C}_{6h}$	1, 2, 2_z, $\overline{1}$	$6/m \rhd 6 \rhd \ldots$
622	$\mathcal{D}_6$	1, 3, 2_z, 2_{110}	$622 \rhd 6 \rhd \ldots$
$6mm$	$\mathcal{C}_{6v}$	1, 3, 2_z, m_{110}	$6mm \rhd 6 \rhd \ldots$
$\overline{6}2m$	$\mathcal{D}_{3h}$	1, 3, m_z, 2_{110}	$\overline{6}2m \rhd \overline{6} \rhd \ldots$
$6/mmm$	$\mathcal{D}_{6h}$	1, 3, 2_z, 2_{110}, $\overline{1}$	$6/mmm \rhd 622 \rhd \ldots$

Composition series of point group $6/mmm$ and its subgroups, see also Fig. 1.5.2. For the longer composition series only the first members are listed. The complete series can be composed step by step using the previous composition series.

way. In *IT*A, the generators are designated by the numbers in front of the corresponding general-position co-ordinate triplets.
The coordinate triplets of the *General position* are obtained by single-sided, (*i.e* left-sided) multiplication of the matrices representing the generators until no new matrices are found. Resulting matrices that differ only by a lattice translation are considered as equal, and the translations parts are chosen such so that the symmetry operations lie within the unit cell.
The generating procedure used in *IT*A highlights important subgroups of space groups as much as possible. For example, once the translation subgroup $\mathcal{T}_\mathcal{G}$ of a space group $\mathcal{G}$ is generated, the process of generation follows step-wise procedure via a chain of normal and maximal subgroups

$$\mathcal{G} \rhd \mathcal{H}_1 \rhd \mathcal{H}_2 \rhd \cdots \rhd \mathcal{T}_\mathcal{G}, \tag{1.5.16}$$

with indices $|\mathcal{H}_i : \mathcal{H}_{i+1}|$ equal to 2 or 3. In other words, each new (non-translational) generator generates a minimal *translationengleiche* or *t*-supergroup $\mathcal{H}_i$ of $\mathcal{H}_{i+1}$ of index 2 or 3.

1.6 Exercises

1.6.1 Matrix calculus in crystallography (brief revision)

- **Exercise** 1.6.1.1. Matrix transposition

  1. Construct the transposed matrix of the (3×1) row matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 3 & 4 \end{pmatrix}$.
  2. Determine which of the following matrices are *symmetric* and which are *skew-symmetric*
  $\boldsymbol{A} = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}; \boldsymbol{B} = \begin{pmatrix} 3 & 4 \\ -4 & 1 \end{pmatrix}; \boldsymbol{C} = \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}; \boldsymbol{D} = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}; \boldsymbol{E} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix};$
  $\boldsymbol{F} = \begin{pmatrix} 2 \end{pmatrix}; \boldsymbol{G} = \begin{pmatrix} 0 & 1 & -2 \\ -1 & 0 & 3 \\ 2 & -3 & 0 \end{pmatrix}; \boldsymbol{H} = \begin{pmatrix} 3 & 2 \\ 2 & 1 \\ 1 & 0 \end{pmatrix}; \boldsymbol{J} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$

- **Exercise** 1.6.1.2. Matrix addition and subtraction

  1. Find $3\boldsymbol{A}$-$2\boldsymbol{B}$, where $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 3 & 0 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 1 & 3 \\ 0 & -4 \end{pmatrix}$.
  2. Show that the sum of any matrix and its transposed is a symmetric matrix, *i.e.* $(\boldsymbol{A} + \boldsymbol{A}^T)^T = \boldsymbol{A} + \boldsymbol{A}^T$.
  3. Show that the difference of any matrix and its transposed is a skew-symmetric matrix, *i.e.* $(\boldsymbol{A} - \boldsymbol{A}^T)^T = -(\boldsymbol{A} - \boldsymbol{A}^T)$.

- **Exercise** 1.6.1.3. Matrix multiplication

  1. Find the products $\boldsymbol{AB}$ and $\boldsymbol{BA}$ if they exists, where $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 3 & -4 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 3 & -2 & 2 \\ 1 & 0 & -1 \end{pmatrix}$.
  2. Find the matrix products $\boldsymbol{AB}$ and $\boldsymbol{BA}$ of the row vector $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$ and the column vector $\boldsymbol{B} = \begin{pmatrix} -2 \\ 4 \\ 1 \end{pmatrix}$.
  3. Prove that $\boldsymbol{A}(\boldsymbol{BC})$=$(\boldsymbol{AB})\boldsymbol{C}$ where $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix}$, $\boldsymbol{B} = \begin{pmatrix} 1 & 0 & -1 \\ 2 & 1 & 0 \end{pmatrix}$ and $\boldsymbol{C} = \begin{pmatrix} 1 & -1 \\ 3 & 2 \\ 2 & 1 \end{pmatrix}$.

- **Exercise** 1.6.1.4. Trace and determinant of a matrix

  1. Find the values of the traces and the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$ where $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 0 & 4 & 2 \\ 4 & -2 & -1 \\ 5 & 1 & 3 \end{pmatrix}$.
  2. Show that $det(\boldsymbol{AB}) = det(\boldsymbol{A})det(\boldsymbol{B})$ where $\boldsymbol{A} = \begin{pmatrix} 3 & 2 \\ 5 & 1 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 1 & 6 \\ 2 & 9 \end{pmatrix}$.

3. Show that $det(\boldsymbol{A}) = det(\boldsymbol{A}^T)$ where $\boldsymbol{A} = \begin{pmatrix} 1 & 1 & 3 \\ 2 & 2 & 2 \\ 3 & 2 & 3 \end{pmatrix}$.

- **Exercise** 1.6.1.5. Inverse of a matrix

1. Show that the matrix $\boldsymbol{B} = 1/3 \begin{pmatrix} 11 & -9 & 1 \\ -7 & 9 & -2 \\ 2 & -3 & 1 \end{pmatrix}$ is the inverse of $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 5 \\ 1 & 5 & 12 \end{pmatrix}$.
2. Determine the inverses of the matrices $\boldsymbol{A} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$; $\boldsymbol{B} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$; $\boldsymbol{C} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$; $\boldsymbol{D} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$; $\boldsymbol{E} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$ and $\boldsymbol{F} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.
3. Given that $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ -1 & 0 & 3 \\ 2 & -1 & 0 \end{pmatrix}$ determine $\boldsymbol{A}^{-1}$.

- **Exercise** 1.6.1.6. Matrix-column presentation of symmetry operations

1. Referred to an 'orthorhombic' coordinate system ($a \neq b \neq c; \alpha = \beta = \gamma = 90$) two symmetry operations are represented by the following matrix-column pairs: $(\boldsymbol{W}_1, \boldsymbol{w}_1) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} \right)$.
   (a) Determine the images X_i of a point $X = \begin{pmatrix} 0.7 \\ 0.31 \\ 0.95 \end{pmatrix}$ under the action of the symmetry operations.
   (b) Can you guess what is the 'geometric nature' of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$?
   (c) Determine the determinant and the trace of $\boldsymbol{W}_1$.
   (d) Determine the sets of fixed points of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$.
2. Consider the matrix-column pairs of the two symmetry operations $(\boldsymbol{W}_1, \boldsymbol{w}_1) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} \right)$.

(a) Determine and compare the matrix-column pairs of the combined symmetry operations: $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{W}_1,\boldsymbol{w}_1)(\boldsymbol{W}_2,\boldsymbol{w}_2)$ and $(\boldsymbol{W},\boldsymbol{w})' = (\boldsymbol{W}_2,\boldsymbol{w}_2)(\boldsymbol{W}_1,\boldsymbol{w}_1)$.

(b) Determine the inverse symmetry operations $(\boldsymbol{W}_1,\boldsymbol{w}_1)^{-1}$ and $(\boldsymbol{W}_2,\boldsymbol{w}_2)^{-1}$.

(c) Determine the inverse symmetry operation $(\boldsymbol{W},\boldsymbol{w})^{-1}$ if $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{W}_1,\boldsymbol{w}_1)(\boldsymbol{W}_2,\boldsymbol{w}_2)$.

3. Consider the matrix-column pairs $(\boldsymbol{A},\boldsymbol{a}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}\right)$ and $(\boldsymbol{B},\boldsymbol{b}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right)$.

(a) What are the matrix-column pairs resulting from: $(\boldsymbol{A},\boldsymbol{a})(\boldsymbol{B},\boldsymbol{b}) = (\boldsymbol{C},\boldsymbol{c})$ and $(\boldsymbol{B},\boldsymbol{b})(\boldsymbol{A},\boldsymbol{a}) = (\boldsymbol{D},\boldsymbol{d})$.

(b) Determine $(\boldsymbol{A},\boldsymbol{a})^{-1}$, $(\boldsymbol{B},\boldsymbol{b})^{-1}$, $(\boldsymbol{C},\boldsymbol{c})^{-1}$ and $(\boldsymbol{D},\boldsymbol{d})^{-1}$. What is $(\boldsymbol{B},\boldsymbol{b})^{-1}(\boldsymbol{A},\boldsymbol{a})^{-1}$?

1.6.2 Space-group symmetry data

- **Exercise** 1.6.2.1. Matrix-column presentation of symmetry operations

1. Referred to an 'orthorhombic' coordinate system ($a \neq b \neq c; \alpha = \beta = \gamma = 90$) two symmetry operations are represented by the following matrix-column pairs:

$$(\boldsymbol{W}_1,\boldsymbol{w}_1) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right) \text{ and } (\boldsymbol{W}_2,\boldsymbol{w}_2) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}\right).$$

(a) Determine the images X_i of a point $X = \begin{pmatrix} 0.7 \\ 0.31 \\ 0.95 \end{pmatrix}$ under the action of the symmetry operations.

(b) Can you guess what is the 'geometric nature' of $(\boldsymbol{W}_1,\boldsymbol{w}_1)$ and $(\boldsymbol{W}_2,\boldsymbol{w}_2)$?

(c) Determine the determinant and the trace of $\boldsymbol{W}_1$.

(d) Determine the sets of fixed points of $(\boldsymbol{W}_1,\boldsymbol{w}_1)$ and $(\boldsymbol{W}_2,\boldsymbol{w}_2)$.

2. Consider the matrix-column pairs of the two symmetry operations

$$(\boldsymbol{W}_1,\boldsymbol{w}_1) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right) \text{ and } (\boldsymbol{W}_2,\boldsymbol{w}_2) = \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}\right).$$

(a) Determine and compare the matrix-column pairs of the combined symmetry operations: $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{W}_1,\boldsymbol{w}_1)(\boldsymbol{W}_2,\boldsymbol{w}_2)$ and $(\boldsymbol{W},\boldsymbol{w})' = (\boldsymbol{W}_2,\boldsymbol{w}_2)(\boldsymbol{W}_1,\boldsymbol{w}_1)$.

(b) Determine the inverse symmetry operations $(\boldsymbol{W}_1,\boldsymbol{w}_1)^{-1}$ and $(\boldsymbol{W}_2,\boldsymbol{w}_2)^{-1}$.

(c) Determine the inverse symmetry operation $(\boldsymbol{W},\boldsymbol{w})^{-1}$ if $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{W}_1,\boldsymbol{w}_1)(\boldsymbol{W}_2,\boldsymbol{w}_2)$.

3. Consider the matrix-column pairs $(\boldsymbol{A},\boldsymbol{a}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}\right)$ and $(\boldsymbol{B},\boldsymbol{b}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right)$.

(a) What are the matrix-column pairs resulting from: $(\boldsymbol{A},\boldsymbol{a})(\boldsymbol{B},\boldsymbol{b}) = (\boldsymbol{C},\boldsymbol{c})$ and $(\boldsymbol{B},\boldsymbol{b})(\boldsymbol{A},\boldsymbol{a}) = (\boldsymbol{D},\boldsymbol{d})$.

(b) Determine $(\boldsymbol{A}, \boldsymbol{a})^{-1}$, $(\boldsymbol{B}, \boldsymbol{b})^{-1}$, $(\boldsymbol{C}, \boldsymbol{c})^{-1}$ and $(\boldsymbol{D}, \boldsymbol{d})^{-1}$. What is $(\boldsymbol{B}, \boldsymbol{b})^{-1}(\boldsymbol{A}, \boldsymbol{a})^{-1}$?

- **Exercise** 1.6.2.2. Consider the *General position* data given in ITA for the space group

  (a) $Cmm2$ (No. 35):

  1. Characterize geometrically the matrix-column pairs listed under *General position* of the space group $Cmm2$. Compare the results with the data listed under *Symmetry operations*.
  2. Consider the diagram of the symmetry elements of $Cmm2$. Try to determine the matrix-column pairs of the symmetry operations whose symmetry elements are indicated on the unit-cell diagram.
  3. Compare your results with the results of the program `SYMMETRY OPERATIONS` for the geometric interpretation of the matrix-column pairs of the symmetry operations considered in this exercise.

  (b) $P4mm$ (No. 99):

  1. Characterize geometrically the matrix-column pairs listed under *General position* of the space group $P4mm$. Compare the results with the data listed under *Symmetry operations*.
  2. Consider the diagram of the symmetry elements of $P4mm$. Try to determine the matrix-column pairs of the symmetry operations whose symmetry elements are indicated on the unit-cell diagram.
  3. Compare your results with the results of the program `SYMMETRY OPERATIONS` for the geometric interpretation of the matrix-column pairs of the symmetry operations considered in this exercise.

  Attachments: Copies of the ITA pages with the space-group data of $Cmm2$, No. 35.
  Copies of the ITA pages with the space-group data of $P4mm$, No. 99.

- **Exercise** 1.6.2.3. The *General position* of a space group is listed as:
  (1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$
  (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$.

  1. Construct the matrix-column pairs of these 'coordinate triplets'. Write down the corresponding (4×4) matrix representation.
  2. Characterize geometrically the matrices if they refer to a monoclinic basis with unique axis b (type of operation, glide (screw) component, fixed points, nature and location of the symmetry element).
  3. Use the program `SYMMETRY OPERATIONS` of BCS for the geometric interpretation of the matrix-column pairs of the symmetry operations.

- **Exercise** 1.6.2.4. Determine the orientation and location of the three mutually perpendicular 2-fold rotation axes in the space groups $P222$, $P222_1$, $P2_12_12$ y $P2_12_12_1$.

- **Exercise** 1.6.2.5. Consider the special Wyckoff positions of the the space group $P4mm$ (No. 99)

  1. Determine the site-symmetry groups of Wyckoff positions $1a$ and $1b$. Compare the results with the listed data of $P4mm$ in ITA .
  2. The coordinate triplets $(x, 1/2, z)$ and $(1/2, x, z)$, belong to Wyckoff position $4f$. Compare their site-symmetry groups.
  3. Compare your results with the output of the BCS program `WYCKPOS` for the space group $P4mm$.

4. Use the option *Non-conventional settings* of the program `WYCKPOS` to determine the coordinate triplets of the Wyckoff positions of the space group $P4mm$ referred to a non-conventional setting with the four-fold rotation axes parallel to **a** axis.

Attachments: Copies of the *IT*A pages with the space-group data of $P4mm$, No. 99.

- **Exercise** 1.6.2.6. The following matrix-column pairs ($\boldsymbol{W}$, $\boldsymbol{w}$) are determined with respect to a basis (**a**,**b**,**c**): (1) x, y, z (2) $\bar{x}, y+\frac{1}{2}, \bar{z}+\frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$.
  - Determine the corresponding matrix-column pairs ($\boldsymbol{W}'$, $\boldsymbol{w}'$) with respect to the basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, with $\boldsymbol{P}=$ **c**,**a**,**b**.
  - The coordinates of a point $X = \begin{pmatrix} 0.70 \\ 0.31 \\ 0.95 \end{pmatrix}$ are determined with respect to the basis (**a**,**b**,**c**). What would be the coordinates X' referred to the basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$?

- **Exercise** 1.6.2.7. *IT*A -conventional settings of space groups

  1. Consider the space group $P2_1/c$ (No. 14). Show that the relation between the *General* and *Special position* data of $P112_1/a$ (setting *unique axis c*) can be obtained from the data $P12_1/c1$ (setting *unique axis b*) applying the transformation $(\mathbf{a}, \mathbf{b}, \mathbf{c})_c = (\mathbf{a}, \mathbf{b}, \mathbf{c})_b \boldsymbol{P}$, with $\boldsymbol{P}=$ **c**,**a**,**b**.
  2. Use the BCS retrieval tools `GENPOS` (generators and general positions) and `WYCKPOS` (Wyckoff positions for accessing *IT*A data. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in *IT*A (*cf.* Table 4.3.2.1).

Attachments: Copies of the *IT*A pages with the space-group data of $P2_1/c$ (No. 14).

- **Exercise** 1.6.2.8. *IT*A and Non-conventional settings of space groups

  1. Use the BCS retrieval tools `GENPOS` (generators and general positions), `WYCKPOS` (Wyckoff positions and `HKLCOND` (reflection conditions) for accessing *IT*A data. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in *IT*A (*cf.* Table 4.3.2.1).
  2. Consider the General position data of the space group $Im\bar{3}m$ (No. 229). Using the option $Non-conventional\,setting$ obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis $(\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)$, applying the transformation $\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p = \frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$ (where $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is the conventional basis).

1.6.3 Group-subgroup relations of space groups

- **Exercise** 1.6.3.1. Construct the diagram of the *t*-subgroups of $P4mm$ using the 'analogy' with the subgroup diagram of the group $4mm$, *cf.* Exercise **??**. Give the standard Hermann-Mauguin symbols of the t -subgroups of $P4mm$.

- **Exercise** 1.6.3.2. The retrieval tool `MAXSUB` gives an access to the database on maximal subgroups of space groups as listed in *IT*A1. Consider the maximal subgroups of the group $P4mm$, (No. 99) and compare them with the maximal subgroups of $P4mm$ derived in Problem 1.6.3.1 (*IT*A *Exercises*). Comment on the differences, if any.

- **Exercise** 1.6.3.3. Study the group–subgroup relations between the groups $\mathcal{G} = P4_12_12$, No. 92, and $\mathcal{H} = P2_1$, No. 4 using the program `SUBGROUPGRAPH`. Consider the cases with specified (*e.g.* $[i] = 4$) and unspecified index of the group-subgroup pair.

- **Exercise** 1.6.3.4. *Translationengleiche* subgroups of $P4mm$

  (a) Explain the difference between the *contracted* and *complete* graphs of the t-subgroups of $P4mm$ (No. 99) obtained by the program `SUBGROUPGRAPH`. Compare the complete graph with the results of Problems **??**. and 1.6.3.1 of *IT*A *Exercises*.

  (b) Explain why the t-subgroup graphs of all 8 space groups from No. 99 ($P4mm$) to No. 106 ($P4_2bc$) have the same 'topology' (*i. e.* the same type of 'family tree'), only the corresponding subgroup entries differ.

- **Exercise** 1.6.3.5. Domain-structure analysis

  Determine the type and number of domain states in structural phase transitions specified by:

  1. High-symmetry phase: $P2/m$
     Low-symmetry phase: $P1$ with small unit-cell deformation;
  2. High-symmetry phase: $P2/m$
     Low-symmetry phase: $P1$ with duplication of the unit cell;
  3. High-symmetry phase: $P4mm$
     Low-symmetry phase: $P2$ of index 8;
  4. High-symmetry phase: $P4_2bc$
     Low-symmetry phase: $P2_1$ of index 8.

- **Exercise** 1.6.3.6. Phase transitions in $BaTiO_3$

  The crystal structure of $BaTiO_3$ is of perovskite type. Above 120C $BaTiO_3$ has the ideal paraelectric cubic structure (space group $Pm\bar{3}m$) shown in Figure 1.1. Below 120C $BaTiO_3$ assumes three structures with slightly deformed unit cells, all three being ferroelectric with different directions of the axis of spontaneous polarisation (polar axis). The three ferroelectric polymorphs differ in the direction of displacement of the Ti-atoms from the centres of the octahedra (and the accompanying lattice distortion):

  (a) No displacement: cubic structure

  (b) Displacement parallel to a cube edge: $< 100 >$, symmetry group $P4mm$;

  (c) Displacement parallel to face diagonal of the cube:$< 110 >$, symmetry group $Amm2$;

  (d) Displacement parallel to a body diagonal of the cube: $< 111 >$, symmetry group $R3m$.

  (i) Which subgroup indices do the three space groups of the ferroelectric polymorphs display with respect to the cubic group $Pm\bar{3}m$?

  (ii) How many orientation states of the twin domains occur for each polymorph? Which mutual orientation do the domains exhibit for case (b)?

- **Exercise** 1.6.3.7. $SrTiO_3$ has the cubic perovskite structure, space group $Pm\bar{3}m$. Upon cooling below 105K, the coordination octahedra are mutually rotated and the space group is reduced to $I4/mcm$; c is doubled and the unit cell is increased by the factor of four. Can we expect twinned crystals of the low symmetry form? If so, how many kinds of domains?

  Determine the number and type of domains of the low-symmetry form of $SrTiO_3$ using the computer tools of the Bilbao Crystallographic server.

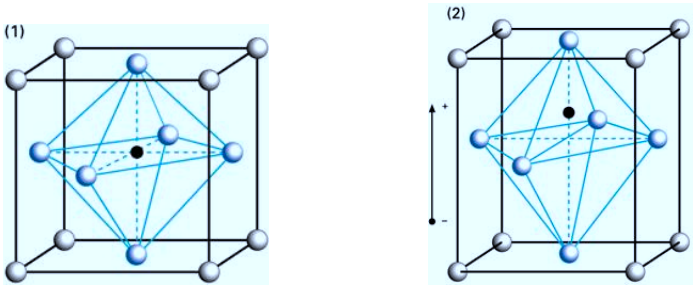


Figure 1.1: (1) Perovskite structure (undistorted); (2) Distorted perovskite structure: Ti displacements and lattice distortion parallel to a cube edge, and the related dipole generation in $BaTiO_3$

- **Exercise** 1.6.3.8. Study the splittings of the Wyckoff positions for the group-subgroup pair $P4mm$ (No. 99)> Cm (No. 4) of index 4 by the program `WYCKSPLIT`.
- **Exercise** 1.6.3.9. Consider the group–supergroup pair $\mathcal{H} < \mathcal{G}$ with $\mathcal{H} = P222$, No. 16, and the supergroup $\mathcal{G} = P422$, No. 89, of index $[i] = 2$. Using the program `MINSUP` determine all supergroups $P422$ of $P222$ of index $[i] = 2$. How does the result depend on the normalizer of the supergroup and/or that of the subgroup.

1.6.4 Crystal-structure descriptions

- **Exercise** 1.6.4.1. Structure descriptions for different space-group settings

Problem 1.6.4.1A Scheelite ($CaWO_4$)

Scheelite ($CaWO_4$) is a mineral that crystallizes in the space group $I4_1/a$ (No. 88). In the *Inorganic Crystal Structure Database* the following two descriptions of $CaWO_4$ can be found:

# (a) Origin choice 1						# (b) Origin choice 2					
88						88					
5.243	5.243	11.376	90	90	90	5.243	5.243	11.376	90	90	90
3						3					
Ca	1	4*b*	0.0000	0.0000	0.5000	Ca	1	4*b*	0.0000	0.2500	0.6250
W	1	4*a*	0.0000	0.0000	0.0000	W	1	4*a*	0.0000	0.2500	0.1250
O	1	16*f*	0.2413	0.1511	0.0861	O	1	16*f*	0.1504	0.0085	0.2111

(1) Compare the two structure descriptions using the program `SETSTRU`.

(2) Use the program `TRANSTRU` to compare these two structure descriptions. Use as transformation matrix the origin shift $\boldsymbol{p} = 0, 1/4, 1/8$ to transform the structure described in origin choice 1 into origin choice 2.

Hint: In order to compare the different data, the parameters of Structure (a) are to be transformed to 'origin at center $2/m$', i.e. ORIGIN CHOICE 2.

Problem 1.6.4.1B Zircon $ZrSiO_4$ (Wondratschek, 2002)

(a) In R. W. G. Wyckoff, *Crystal structures*, vol. **II**, Ch. VIII, one finds the important mineral zircon $ZrSiO_4$ and a description of its crystal structure. Many rare-earth phosphates, arsenates, and vanadates belong to the same structure type.

Structural data: Space group $I4_1/amd = D_{4h}^{19}$, No. 141;
lattice constants a = 6.60 Å; c = 5.88 Å.

The origin choice is not stated explicitly. However, Wyckoff's *Crystal Structures* started to appear in 1948, when there was one conventional origin only (the later ORIGIN CHOICE 1, *i. e.* **Origin** at $\bar{4}m2$).

$Zr:$ (a) $0,0,0;\ 0,\frac{1}{2},\frac{1}{4};\ \frac{1}{2},0,\frac{3}{4};\ \frac{1}{2},\frac{1}{2},\frac{1}{2};$
$Si:$ (b) $0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4};\ \frac{1}{2},0,\frac{1}{4};\ \frac{1}{2},\frac{1}{2},0;$
$O:$ (h) $(0,u,v;\ 0,\bar{u},v;\ u,0,\bar{v};\ \bar{u},0,\bar{v};\ 0,\frac{1}{2}+u,\frac{1}{4}-v;\ 0,\frac{1}{2}-u,\frac{1}{4}-v;$
$\bar{u},\frac{1}{2},v+\frac{1}{4};\ u,\frac{1}{2},v+\frac{1}{4};)$ [and the same with $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$].

The parameters u and v are listed with $u = 0.20$ and $v = 0.34$.

(b) In the *Structure Reports*, vol. **22**, (1958), p. 314 one finds:

'a = 6.6164(5) Å, c = 6.0150(5) Å'
'Atomic parameters. Origin at center $(2/m)$ at $0, \frac{\bar{1}}{4}, \frac{1}{8}$ from $\bar{4}m2$.'
'Oxygen: (0, y, z) with $y = 0.067$, $z = 0.198$.'

Compare the two structure descriptions and check if they belong to the same structure type. Which of the structure tools of the Bilbao Crystallographic Server could help you to solve the problem?

*Hint:*In order to compare the different data, the parameters of Wyckoff's book are to be transformed to 'origin at center $2/m$', *i. e.* ORIGIN CHOICE 2.

- **Exercise** 1.6.4.2. Equivalent structure descriptions

(a) CsCl is cubic, space group $Pm\bar{3}m$, with the following co-ordinates

Atom	Wyckoff position	Coordinate triplets x	y	z
Cl	$1a$	0.0	0.0	0.0
Cs	$1b$	0.5	0.5	0.5

How many equivalent sets of co-ordinates can be used to describe the structure? What are their co-ordinates?

Hint: The number of different equivalent descriptions of CsCl is equal to the index of its space group $Pm\bar{3}m(\mathbf{a},\mathbf{b},\mathbf{c})$ in the Euclidean normalizer $Im\bar{3}m(\mathbf{a},\mathbf{b},\mathbf{c})$, *i.e.* $[i] = 2$. The two different descriptions are generated by the coset representatives of the decomposition of the normalizer with respect to the space group.

(b) $P(C_6C_5)_4[MoNCl_4]$ is tetragonal, space group $P4/n$, with the following co-ordinates:

Atom	Wyckoff position	Coordinate triplets x	y	z
P	$2b$	0.25	0.75	0
Mo	$2c$	0.25	0.25	0.121
N	$2c$	0.25	0.25	−0.093
C1	$8g$	0.362	0.760	0.141
C2	$8g$	0.437	0.836	0.117
Cl	$8g$	0.400	0.347	0.191

(H and C3 to C6 omitted)

How many equivalent sets of co-ordinates can be used to describe the structure? What are their co-ordinates?

Hint: The number of different equivalent descriptions of $P(C_6C_5)_4[MoNCl_4]$ is equal to the index of its space group $P4/n$ in the Euclidean normalizer. The different descriptions are generated by the coset representatives of the decomposition of the normalizer with respect to the space group. In the special case of $P(C_6C_5)_4[MoNCl_4]$ such equivalent descriptions can be generated, for example, by the translations $t(0, 0, 1/2)$ and $t(1/2, 1/2, 0)$, and by a reflection through a mirror plane at (x, x, z) represented by the coordinate triplet (y, x, z).

- **Exercise** 1.6.4.3. Isoconfigurational structure types (Koch & , Fischer, 2002)

  Do the following three structures belong to the same structure type? Try to find analogous coordinate descriptions for all three crystal structures.

  1. $KAsF_6$ (ICSD: 59413)

     Unit Cell 7.348(1) 7.348(1) 7.274(8) 90. 90. 120

     Space group R-3h

Atom	Wyckoff position	Coordinate triplets x	y	z
K	$3b$	0.33333	0.66667	0.166667
As	$3a$	0	0	0
F	$18f$	0.1292(2)	0.2165(2)	0.1381(2)

  2. $BaIrF_6$ (ICSD: 803188)

     Unit Cell 7.3965(1) 7.3965(1) 7,2826(1) 90. 90. 120

     Space group R-3h

Atom	Wyckoff position	Coordinate triplets x	y	z
Ba	$3b$	0.33333	0.6666	0.166666
Ir	$3a$	0	0	0
F	$18f$	0.0729(2)	0.2325(2)	0.1640(2)

3. $BaSnF_6$ (ICSD: 33788)

   Unit Cell 7.4279(2) 7.4279(2) 7.418(2) 90. 90. 120

   Space group R-3h

Atom	Wyckoff position	Coordinate triplets x	y	z
Ba	$3a$	0	0	0
Sn	$3b$	0	0	0.5
F	$18f$	0.2586(3)	0.8262(3)	0.0047(3)

   Hint: Consider the Euclidean normalizer of symmetry group $R\overline{3}$(hex) of $KAsF_6$. The number of different equivalent descriptions of $KAsF_6$ is equal to the index of its space group in the Euclidean normalizer. The different descriptions are generated by the coset representatives of the decomposition of the normalizer with respect to the space group. In the special case of $KAsF_6$ such equivalent descriptions can be generated, for example, by the translation $t(0, 0, 1/2)$, by a reflection through a mirror plane at $(x, -x, z)$ represented by the coordinate triplet $(-y, -x, z)$, etc.

- **Exercise** 1.6.4.4. Crystal structure descriptions

  In Inorganic Crystal Structure Database can be found several structure data sets of ϵ-Fe_2O_3, all of them of symmetry $Pna2_1$ (No.33). Compare the two structure descriptions listed in the *Exercise Data* file and check if they belong to the same structure type.

Chapter 2

The irreps of the crystallographic point groups

In this chapter the representations of the crystallographic point groups are dealt with. Basic definitions and lemmata of the representation theory of finite groups are presented in Section 2.1. Section 2.2 contains the derivation of the irreps of cyclic and non-cyclic Abelian groups. In Section 2.3 the direct products of $\mathcal{C}_2$ with the 'basic' groups of Section 2.4 are dealt with. Further developments of representation theory necessary for the development of a general procedure for the irrep derivation is found in Chapter 2.5.

2.1 Representations

Definition (D 2.1.0.1) A group $\mathcal{H}$ of concrete elements (mappings, permutations, matrices, *etc.*) is called a *representation* $\mathbf{D}$ (*sensu lato*) of the (abstract) group $\mathcal{G}$ if $\mathcal{H}$ is a homomorphic image of $\mathcal{G}$. A representation is called *faithful* if the homomorphism is one-to-one, *i. e.* is an isomorphism.

■ Example. The 24 symmetry operations of a regular tetrahedron, the 24 permutations of its 4 vertices, and the 24 matrices of the 'general position' of space group $P\bar{4}3m$, No. 215 of IT A are faithful representations of the group $\mathcal{T}$, the 'tetrahedral group'. ■

If the elements are matrices with the combination law of matrix multiplication then the representation is called a *representation* (*sensu stricto*) or simply 'representation' and is here abbreviated as *rep*. Only such reps by matrices are dealt with in this manuscript.
The rank of the matrices is called the *dimension* of the rep.

For convenience we repeat 3 important properties of reps:

1. Let $\mathcal{G}$ be a group and $\mathcal{H}$ a rep of $\mathcal{G}$. If $g_m \rightarrow h_m$, $g_n \rightarrow h_n$, and $g_m g_n = g_{mn} \rightarrow h_{mn}$, then $h_m h_n = h_{mn}$ for all g_m, $g_n \in \mathcal{G}$, *i. e.* the product of the images is equal to the image of the product.

2. A normal subgroup of $\mathcal{G}$, called the *kernel* $\mathcal{K} \trianglelefteq \mathcal{G}$ is mapped onto the unit element $e \in \mathcal{H}$.

3. The group $\mathcal{H}$ is a faithful rep of the factor group $\mathcal{G}/\mathcal{K}$ but not necessarily isomorphic to a subgroup of $\mathcal{G}$.

Lemma 2.1.1 A rep of every group $\mathcal{G}$ is the *identity rep* which assigns the (one-dimensional matrix) 1 to each element of $\mathcal{G}$. It is also called the 'trivial rep'.

2.1.1 Matrices

A matrix rep forms a group. Therefore, its matrices $\boldsymbol{A}$ are regular square matrices with finite orders and $|\det \boldsymbol{A}| = 1$. An example for a matrix of infinite order is $\boldsymbol{B} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$.

Definition (D 2.1.1.1) Equivalent matrices. Two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are called *equivalent* if there is a regular matrix $\boldsymbol{X}$ with $\boldsymbol{X}^{-1}\,\boldsymbol{A}\,\boldsymbol{X} = \boldsymbol{B}$.

By this definition the set of all regular matrices is distributed to equivalence classes. Equivalent matrices have the same order and the same eigenvalues, in particular the same trace and determinant. One can understand equivalent matrices as different descriptions of the same mapping but referred to different bases. Therefore, they are considered not to be essentially different.

Definition (D 2.1.1.2) A matrix $\boldsymbol{A}$ is called *reducible* if it is equivalent to a matrix of the form $\begin{pmatrix} \boldsymbol{R}_1 & \boldsymbol{S} \\ \boldsymbol{O} & \boldsymbol{R}_2 \end{pmatrix}$. It is called *fully reducible* if $\boldsymbol{S} = \boldsymbol{O}$ is the matrix consisting only of zeroes.

Lemma 2.1.2 Any matrix of finite order is fully reducible to components of dimension 1.

■ Example.The matrix $\boldsymbol{B} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ is reduced but is not fully reducible.

This is no contradiction because $\boldsymbol{B}$ is of infinite order. ■

2.1.2 General remarks on representations

Every group $\mathcal{G}$ has infinitely many reps. How can one get an overview on them ?
In the same way as for matrices the concepts: *equivalent*, *reducible*, and *fully reducible* can be defined also for sets of matrices, including matrix groups. Here only the definition for the equivalence of reps of groups is formulated. The other definitions are analogous.

Definition (D 2.1.2.1) Equivalent reps. Two reps $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ of a group $\mathcal{G}$ are called *equivalent* if there is a regular matrix $\boldsymbol{X}$ which transforms the matrices $\boldsymbol{A}_1(g_k) \in \mathbf{D}^{(1)}$ simultaneously to $\boldsymbol{A}_2(g_k) \in \mathbf{D}^{(2)}$: $\boldsymbol{X}^{-1}\,\boldsymbol{A}_1(g_k)\,\boldsymbol{X} = \boldsymbol{A}_2(g_k)$ for all elements $g_k \in \mathcal{G}$.

One can understand equivalent reps as different descriptions of the same group of mappings but referred to different bases. Therefore, they are considered not to be essentially different.

Lemma 2.1.3 Each rep of a finite group is equivalent to a rep by unitary matrices.

Other than a single matrix, a rep is not necessarily reducible or fully reducible to components of dimension 1.

Definition (D 2.1.2.2) A set of matrices is called *irreducible* if it is neither reducible or fully reducible.

Lemma 2.1.4 Each rep of a finite group is either fully reducible or irreducible. A rep $\mathbf{D}$ which is fully reduced into the reps $\mathbf{D}^{(1)}$ with matrices $\{\boldsymbol{D}^{(1)}(g_k)\}$ and $\mathbf{D}^{(2)}$ with matrices $\{\boldsymbol{D}^{(2)}(g_k)\}$ is called the *direct sum* $\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}$ of the reps $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$. With $\mathbf{D}$ also $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are reps of $\mathcal{G}$.

The reduction can be continued until $\mathbf{D}$ is fully reduced into irreducible constituents $\mathbf{D}^{(i)}$. Then the number n of irreducible constituents in $\mathbf{D}$ is called the *length of the reduction*. The number of occurences of an irreducible constituent $\mathbf{D}^{(i)}$ in the reduction of $\mathbf{D}$ is called its *multiplicity* m_i. Different reductions of a rep have the same length, the same irreducible constituents up to the sequence and equivalence, and the

same multiplicities. A fully reducible rep is determined by its irreducible constituents up to equivalence.

2.1.3 Irreducible representations (irreps)

The number of irreps of a finite group is relatively small; it is strongly restricted by two lemmata which here can be only stated. They are more extensively dealt with in DP.

Lemma 2.1.5 The number of different irreps of a group $\mathcal{G}$ is equal to the number of conjugacy classes of $\mathcal{G}$.

The immediate consequence of this lemma is:

1. The number of irreps of an Abelian group $\mathcal{G}$ is equal to the order of $\mathcal{G}$ because each element $g \in \mathcal{G}$ forms a conjugacy class for itself.

2. The number of irreps of a non-Abelian group $\mathcal{G}$ is smaller than the order of $\mathcal{G}$.

Lemma 2.1.6 The sum of the squares of the dimensions of the different irreps of a group $\mathcal{G}$ is equal to the order of the group: $|\mathcal{G}| = n_1^2 + n_2^2 + \ \ldots\ n_r^2$.

For small group orders $|\mathcal{G}|$ these two lemmata determine the number and the dimensions of the irreps uniquely. However, the 10 irreps of the group $O \times \mathcal{C}_2$ of order 48 might be of dimensions $6+2+1+1+1+1+1+1+1+1$ or $5+3+2+2+1+1+1+1+1+1$ or $4+4+3+1+1+1+1+1+1+1$ or $4+3+2+2+2+2+2+1+1+1$ or $3+3+3+3+2+2+1+1+1+1$ if the structure of the group is not taken into consideration.

A number of crystallographic point groups are direct products of groups, see Table 1.5.1 on p. 16. For the construction of their irreps, the following theorem is very useful.

Lemma 2.1.7 The irreps $\mathbf{D}^{(ij)}(\mathcal{G})$ of the direct product of two groups $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ can be constructed from the irreps $\mathbf{D}^{(i)}(\mathcal{H}_1)$ and $\mathbf{D}^{(j)}(\mathcal{H}_2)$ in the following way: $\mathbf{D}^{(ij)}(\mathcal{G}) = \mathbf{D}^{(i)}(\mathcal{H}_1) \otimes \mathbf{D}^{(j)}(\mathcal{H}_2)$, with the elements $D^{(ij)}(g)_{pq;rs} = D^{(i)}(h_1)_{pr}\, D^{(j)}(h_2)_{qs}$ where $g = h_1\, h_2$. The indices p and r run from 1 to $\dim(\mathbf{D}^{(i)}(\mathcal{H}_1))$; the indices q and s run from 1 to $\dim(\mathbf{D}^{(j)}(\mathcal{H}_2))$. Thus, the dimension of the irrep of $\mathcal{G}$ is equal to the product of the dimensions of the irreps of $\mathcal{H}_1$ and $\mathcal{H}_2$. All irreps of $\mathcal{G}$ are obtained in this way if $\mathbf{D}^{(i)}(\mathcal{H}_1)$ and $\mathbf{D}^{(j)}(\mathcal{H}_2)$ run through all irreps of $\mathcal{H}_1$ and $\mathcal{H}_2$.

■ Example. The *direct product* (or *Kronecker product*) $\boldsymbol{A}\otimes\boldsymbol{B}$ of the two matrices $\boldsymbol{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$ can be expressed by the

super matrix $\boldsymbol{A} \otimes \boldsymbol{B} = \begin{pmatrix} 0\,\boldsymbol{B} & (-1)\,\boldsymbol{B} \\ 1\,\boldsymbol{B} & 0\,\boldsymbol{B} \end{pmatrix} = \left(\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \end{array}\right)$. ■

2.2 The irreps of Abelian groups

Because finite Abelian groups are either cyclic groups or isomorphic to direct products of cyclic groups, their irreps can be easily determined, once the irreps of the cyclic groups are known.

2.2.1 The irreps of cyclic groups

Lemma 2.2.1 The n irreps of a cyclic group $\mathcal{C}_n = \langle g \rangle = \{e,\ g,\ g^2,\ \ldots\ ,\ g^{n-1}\}$ are given by the formula $\mathbf{D}^{(p)}(g^m) = [\exp(2\,\pi\,i\,(p-1)/n)]^m = \exp(2\,\pi\,i\,m(p-1)/n),\ m,\ p = 1,\ 2,\ \ldots\ , n.$

Crystallographic examples are $\mathcal{C}_1,\ \mathcal{C}_2, \mathcal{C}_3,\ \mathcal{C}_4,$ and $\mathcal{C}_6$.

■ Examples.

The group table for $\mathcal{C}_1$ is trivial. From it the table of irreps

$\mathcal{C}_1$	e
A	1

results.

The group table for $\mathcal{C}_2$ is

$\mathcal{C}_2$	e	a
e	e	a
a	a	e

; the table of irreps is

$\mathcal{C}_2$	e	a
$\mathbf{D}^{(1)}$	1	1
$\mathbf{D}^{(2)}$	1	-1

.

The irrep $\mathbf{D}^{(1)}$ is called **A**, the irrep $\mathbf{D}^{(2)}$ is **B**, see Altmann & Herzig (1994). ■

2.2.2 The irreps of direct products of cyclic groups

Each Abelian group is the direct product of cyclic groups. Because the irreps of cyclic group are one-dimensional, the formula for the direct product of irreps in lemma 2.1.7 simplifies considerably. Consider $\mathcal{G} = \mathcal{C}_r \otimes \mathcal{C}_s$, where $\mathcal{C}_r = \langle a \rangle$ and $\mathcal{C}_s = \langle b \rangle$ are cyclic groups of orders r and s. Then the irreps of the generators of group $\mathcal{G}$ are given by

$$\boldsymbol{D}^{(pq)}(a,\, e) = [\exp\, 2\pi\, i\,(p-1)/r] \text{ and } \boldsymbol{D}^{(pq)}(e,\, b) = [\exp\, 2\pi\, i\,(q-1)/s]$$

which are obtained from the general element

$$\boldsymbol{D}^{(pq)}(a^m,\, b^n) = [\exp\, 2\pi\, i\,(p-1)/r]^m\, [\exp\, 2\pi\, i\,(q-1)/s]^n \text{ of } \mathcal{G} \text{ by } n = s \text{ and } m = r.$$

The general element $\boldsymbol{D}^{(pq)}(a^m,\, b^n)$ can be expressed by
$\exp\, 2\pi\, i\, m\,(p-1)/r\, \exp\, 2\pi\, i\, n\,(q-1)/s = \exp\, 2\pi\, i(m\,(p-1)/r\, +\, n\,(q-1)/s),$
where $m,\, p = 1,\ \ldots\ , r$ and $n,\, q = 1,\ \ldots\ , s$.

As a simple illustration of this general result one can consider the irreps of the group $\mathbf{D}_2 = \mathbf{C}_2 \times \mathbf{C}_2$. Its irreps will be dealt with in an exercise.

2.3 The irreps of direct products with the group $\mathcal{C}_2$

All point groups which are direct products and play a role in 3-dimensional crystallography are direct products with the group $\mathcal{C}_2$, see Table 1.5.1 on p. 16. As we have seen, the group $\mathcal{C}_2$ has two 1-dimensional irreps with coefficients ± 1.

Let $\mathcal{G} = \mathcal{H} \times \mathcal{C}_2$ and $\mathbf{D}^{(j)}(\mathcal{H})$ be the irreps of $\mathcal{H}$. Then, each irrep $\mathbf{D}^{(j)}$ of $\mathcal{H}$ gives rise to two irreps of $\mathcal{G}$ which are often designated by $\mathbf{D}^{(j)+}$ and $\mathbf{D}^{(j)-}$ or $\mathbf{D}^{(j)\,g}$ and $\mathbf{D}^{(j)\,u}$ ('g' = gerade; 'u' = ungerade).

$\mathcal{H} \times \mathcal{C}_2$	$\mathcal{H}\, e$	$\mathcal{H}\, a$
$\mathbf{D}^{(j)+}$	$\boldsymbol{D}^{(j)}$	$\boldsymbol{D}^{(j)}$
$\mathbf{D}^{(j)-}$	$\boldsymbol{D}^{(j)}$	$-\boldsymbol{D}^{(j)}$

Examples: irreps of centrosymmetric groups, see Figs. 1.5.1 and 1.5.2.

2.4 The irreps of solvable non-Abelian groups

The irreps of crystallographic non-Abelian groups are well known and treated in many books on representation theory. The general approach for their determination is based on the theory of characters.

The irreps of the non-Abelian groups can also be derived using a procedure which is based on the solvability of the crystallographic groups (*cf.* Section 1.5.2). For convenience, we list generating matrices for the irreps of dimension larger than one of the groups $\mathcal{D}_3,\ \mathcal{D}_4,\ \mathcal{T},$ and $\mathcal{O}$ in the conventional crystallographic bases.

$$\mathcal{D}_3 = 3m = 31m;\ \ \mathbf{D}^{(3)} = \mathbf{E}:\ \mathcal{3}_z^+ = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix};\ \boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Referred to a Cartesian basis, the matrices of the 2-dimensional irrep of the group $\mathcal{D}_3$ are generated from

$$\mathcal{D}_3:\ \ \mathbf{D}^{(3)} = \mathbf{E}:\ \mathcal{3}_z^+ = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix};\ \boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

$$\mathcal{D}_4 = 4mm,\ \mathbf{D}^{(5)} = \mathbf{E}:\ \mathcal{2}_z = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix};\ \mathcal{4}_z^+ = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix};\ \boldsymbol{m}_{yz} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$\mathcal{T} = 23,\ \mathbf{D}^{(4)} = \mathbf{T}:\ \mathcal{2}_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};\ \mathcal{2}_y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix};\ \mathcal{3}_{xxx}^+ = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

The two-dimensional irrep $\mathbf{E}$ of $\mathcal{O}$ consists of the same matrices as $\mathbf{D}^{(3)}$ of $\mathcal{D}_3$. Its kernel is the subgroup $\mathcal{D}_2 \lhd \mathcal{O}$. Therefore, the generators $\mathcal{2}_z$ and $\mathcal{2}_y$ are represented by the unit matrix of $\mathbf{D}^{(3)}$. The generator $\mathcal{3}_{xxx}^+$ of $\mathcal{O}$ replaces the generator $\mathcal{3}_z^+$ of $\mathcal{D}_3$, and $\boldsymbol{m}_{xx}$ of $\mathcal{D}_3$ is replaced by $\mathcal{2}_{xx}$ in group 432 or by $\boldsymbol{m}_{xx}$ in group $\overline{4}3m$.

$$\mathcal{O} = 432\ \ \mathbf{D}^{(4)} = \mathbf{T}^{(1)}:\ \mathcal{2}_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};\ \mathcal{2}_y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix};$$

$$\mathcal{3}_{xxx}^+ = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix};\ \mathcal{2}_{xx} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

$$\mathcal{O} = \overline{4}3m,\ \ \mathbf{D}^{(5)} = \mathbf{T}^{(2)}:\ \mathcal{2}_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};\ \ \mathcal{2}_y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix};$$

$$\boldsymbol{3}xxx^{+} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}; \quad \boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

2.5 Further developments of representation theory

2.5.1 Definitions and general procedure

Subduced and induced representations

Let $\mathcal{H}$ be a proper subgroup of a group $\mathcal{G}$: $\mathcal{H} < \mathcal{G}$. Given an irreducible representation (irrep) $\mathbf{D}^{(r)}(\mathcal{G})$ of $\mathcal{G}$, one can construct a representation (rep) of $\mathcal{H}$ by considering only those matrices of $\mathbf{D}^{(r)}(\mathcal{G})$ which belong to elements of $\mathcal{H}$. This procedure is called *subduction*.

Definition (D 2.5.1.1) Consider the set of matrices which form an irrep of $\mathcal{G}$. The set $\{\boldsymbol{D}^{(r)}(\mathsf{g}_i)\} = \mathbf{D}^{(r)}(\mathcal{G}) \downarrow \mathcal{H},\ \mathsf{g}_i \in \mathcal{H}$, is called the *representation of $\mathcal{H}$ subduced from $\mathcal{G}$*.

Remark. The rep $\{\boldsymbol{D}^{(r)}(\mathsf{g}_i)\} = \mathbf{D}^{(r)}(\mathcal{G}) \downarrow \mathcal{H}$ of $\mathcal{H}$ may be irreducible or reducible.

On the other hand, given an irrep $\mathbf{D}^{(j)}(\mathcal{H})$ of $\mathcal{H}$ one can construct a rep of $\mathcal{G}$. This procedure is called *induction*.

Consider the group-subgroup pair $\mathcal{G} > \mathcal{H}$ and the coset decomposition of $\mathcal{G}$ relative to $\mathcal{H}$:

$$\mathcal{G} = \mathsf{g}_1\,\mathcal{H} \cup \mathsf{g}_2\,\mathcal{H} \cup \ \ldots\ \cup \mathsf{g}_r\,\mathcal{H} \qquad \text{with } \mathsf{g}_1 = \mathsf{e}. \tag{2.5.1}$$

The number r of cosets is equal to the index $r = |\mathcal{G} : \mathcal{H}|$ of $\mathcal{H}$ in $\mathcal{G}$.

Let further $\mathbf{D}^{(j)}(\mathcal{H})$ be an irrep of $\mathcal{H}$ of dimension d.

Lemma 2.5.1 The set of $(r\,d \times r\,d)$ matrices

$$\boldsymbol{D}^{Ind}(\mathsf{g})_{mt,ns} = \begin{cases} \boldsymbol{D}^{(j)}(\mathsf{g}_m^{-1}\,\mathsf{g}\,\mathsf{g}_n)_{t,s} & \text{if } \mathsf{g}_m^{-1}\,\mathsf{g}\,\mathsf{g}_n = \mathsf{h} \in \mathcal{H} \\ 0 & \text{if } \mathsf{g}_m^{-1}\,\mathsf{g}\,\mathsf{g}_n \notin \mathcal{H} \end{cases} \tag{2.5.2}$$

for all $\mathsf{g} \in \mathcal{G}$ forms a representation of $\mathcal{G}$.

Definition (D 2.5.1.2) The representation of lemma 2.5.1 of $\mathcal{G}$ is called an *induced rep* of $\mathcal{G}$.

Remark. The matrix elements of $\boldsymbol{D}^{Ind}(\mathsf{g})$ can also be written in the form

$$\boldsymbol{D}^{Ind}(\mathsf{g})_{mt,ns} = \boldsymbol{M}(\mathsf{g})_{m,n}\boldsymbol{D}^{(j)}(\mathsf{h})_{t,s}, \qquad \text{where } \mathsf{g}_m^{-1}\,\mathsf{g}\,\mathsf{g}_n = \mathsf{h}. \tag{2.5.3}$$

The matrix $\boldsymbol{M}(\mathsf{g})$ is the so-called *induction matrix*. It consists of zeroes and ones only and is thus a so-called *monomial matrix*, having exactly one '1' in the mth row and nth column, determined by the condition $\mathsf{g}_m^{-1}\,\mathsf{g}\,\mathsf{g}_n = \mathsf{h} \in \mathcal{H}$. Correspondingly, the matrices $\boldsymbol{D}^{Ind}(\mathsf{g})$ have block structure with exactly one non-zero block in every column and every row, where the block is the matrix $\boldsymbol{D}^{(j)}(\mathsf{h})$, and h is fixed by the above condition.
Equation 2.5.2 is sometimes written in the form

$$\boldsymbol{D}^{Ind}(\mathsf{g}) = \boldsymbol{M}(\mathsf{g}) \otimes \boldsymbol{D}^{(j)}(\mathsf{h}), \tag{2.5.4}$$

where the sign $\otimes$ is used for the construction in equation 2.5.4 although the matrix $\boldsymbol{D}^{(j)}(\mathsf{h})$ is different for different positions in $\boldsymbol{M}$.

Conjugate representations and orbits

In general the induced reps are reducible. However, our aim is to obtain a procedure for the construction of the *irreps* of a group $\mathcal{G}$ from the irreps of one of its subgroups $\mathcal{H} < \mathcal{G}$. For this we consider a pair 'group–normal subgroup' $\mathcal{G} \rhd \mathcal{H}$.

Definition (D 2.5.1.3) The set of matrices $(\mathbf{D}^{(s)}(\mathcal{H}))_g = \{\mathbf{D}^{(s)}(g^{-1}\, h\, g),\ h \in \mathcal{H}\}$, where $g \in \mathcal{G},\ g \notin \mathcal{H}$, forms a rep of $\mathcal{H}$. It is called a representation *conjugate* to $\mathbf{D}^{(s)}(\mathcal{H})$ by $g \in \mathcal{G}$.

The fact that $(\mathbf{D}^{(s)}(\mathcal{H}))_g$ is a rep follows directly from its definition: $(\mathbf{D}^{(s)}(h_1))_g\,(\mathbf{D}^{(s)}(h_2))_g =$
$= \mathbf{D}^{(s)}(g^{-1}\, h\, g)\,\mathbf{D}^{(s)}(g^{-1}\, h_2\, g) = \mathbf{D}^{(s)}(g^{-1}\, h_1\, g\, g^{-1}\, h_2\, g) = \mathbf{D}^{(s)}(g^{-1}\, h_1\, h_2\, g) = (\mathbf{D}^{(s)}(h_1\, h_2))_g$.

The conjugate rep $(\mathbf{D}^{(s)}(\mathcal{H}))_g$ consists of the same set of matrices as $\mathbf{D}^{(s)}(\mathcal{H})$ but possibly assigned to group elements different from those of $\mathbf{D}^{(s)}(\mathcal{H})$. Therefore,

1. the dimensions of $\mathbf{D}^{(s)}(\mathcal{H})$ and $(\mathbf{D}^{(s)}(\mathcal{H}))_g$ are equal;
2. $(\mathbf{D}^{(s)}(\mathcal{H}))_g$ is an irrep if $\mathbf{D}^{(s)}(\mathcal{H})$ is.
3. If $(\mathbf{D}^{(s)}(\mathcal{H}))_g$ is conjugate to $\mathbf{D}^{(s)}(\mathcal{H})$, then these reps may or may not be equivalent.

Definition (D 2.5.1.4) The set of all inequivalent irreps $(\mathbf{D}^{(s)}(\mathcal{H}))_g$, conjugate to $\mathbf{D}^{(s)}(\mathcal{H})$ by all elements $g \in \mathcal{G}$, is called the *orbit* $O(\mathbf{D}^{(s)}(\mathcal{H}))$ of $\mathbf{D}^{(s)}(\mathcal{H})$ relative to $\mathcal{G}$. The number of reps in the orbit is called the *length* L of the orbit $O(\mathbf{D}^{(s)}(\mathcal{H}))$. A rep $\mathbf{D}^{(s)}(\mathcal{H})$ is called *self-conjugate* if the length of its orbit is $L = 1$.

Many of the possible conjugate irreps $\{(\mathbf{D}^{(s)}(\mathcal{H}))_g,\ g \in \mathcal{G}\}$, are equivalent. In particular, two irreps $(\mathbf{D}^{(s)}(\mathcal{H}))_{g_i}$ and $(\mathbf{D}^{(s)}(\mathcal{H}))_{g_i'}$, conjugate to $(\mathbf{D}^{(s)}(\mathcal{H}))$ by elements g_i and g_i' from the same coset of the decomposition of $\mathcal{G}$ relative to $\mathcal{H}$: $g_i' = g_i\, h', h' \in \mathcal{H}$, are equivalent:

$$(\mathbf{D}^{(s)}(h))_{g_i'} = \mathbf{D}^{s}(g_i'^{-1}\, h\, g_i') = \mathbf{D}^{(s)}(h'^{-1}\, g_i^{-1}\, h\, g_i\, h') = \mathbf{D}^{(s)}(h'^{-1})\,\mathbf{D}^{(s)}(g_i^{-1}\, h\, g_i)\,\mathbf{D}^{(s)}(h') =$$
$$= \mathbf{D}^{(s)}(h')^{-1}(\mathbf{D}^{(s)}(h))_{g_i}\mathbf{D}^{(s)}(h'), \text{ for all } h \in \mathcal{H}.$$

Thus, the complete orbit $O(\mathbf{D}^{(s)}(\mathcal{H}))$ relative to $\mathcal{G}$ is obtained already by conjugation with the coset representatives of $\mathcal{G}$ relative to $\mathcal{H}$. However, also irreps conjugate by elements from different cosets of $\mathcal{H}$ relative to $\mathcal{G}$ may be equivalent, see Section (D 2.5.1.4).

By conjugation the complete set of irreps of $\mathcal{H}$ is distributed into orbits relative to $\mathcal{G}$. The orbits are disjoint because each of them contains mutually conjugated irreps of $\mathcal{H}$.

Little groups, allowed irreps, and induction theorem

Given a group $\mathcal{G} \rhd \mathcal{H}$ and an irrep $\mathbf{D}^{(s)}(\mathcal{H})$ of $\mathcal{H}$, one can define the little group $\mathcal{G}^s$ of $\mathbf{D}^{(s)}(\mathcal{H})$: it is the subset of $\mathcal{G}$ that conjugates $\mathbf{D}^{(s)}(\mathcal{H})$ onto an equivalent irrep.

Definition (D 2.5.1.5) The set of all elements $g \in \mathcal{G}$ for which $\mathbf{D}^{(s)}(\mathcal{H})$ is self-conjugate forms a group which is called the *little group* $\mathcal{G}^s \equiv \mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H}))$ relative to $\mathcal{G}$.

Any element $h \in \mathcal{H}$ leaves $\mathbf{D}^{(s)}(\mathcal{H})$ equivalent under conjugation. Thus, $\mathcal{H} < \mathcal{G}^s$ follows. Moreover, $\mathcal{H} \lhd \mathcal{G}^s$ because $\mathcal{H} \lhd \mathcal{G}$ holds: $\mathcal{G} > \mathcal{G}^s \rhd \mathcal{H}$.

When $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H})) = \mathcal{G}$, all conjugate irreps of $\mathbf{D}^{(s)}(\mathcal{H})$ are equivalent. For example, the identity rep is invariant under any conjugation. Therefore, its little group is always $\mathcal{G}$. Also if $\mathcal{H}$ is in the centre of $\mathcal{G}$, then the $\mathcal{G}$ is the little group of every irrep of $\mathcal{H}$. If the little group of $\mathbf{D}^{(s)}(\mathcal{H})$ is the group $\mathcal{H}$ itself, then

the rep of $(\mathbf{D}^{(s)}(\mathcal{H}))_{g_i}$ is non-equivalent to $\mathbf{D}^{(s)}(\mathcal{H})$, if g_i is any coset representative different from the identity element.

The set of non-equivalent irreps belonging to the orbit of $\mathbf{D}^{(s)}(\mathcal{H})$ is formed by the irreps $(\mathbf{D}^{(s)}(\mathcal{H}))_{g_s}$ which are conjugate by the coset representatives $g_s \in \mathcal{G}$ of $\mathcal{G}$ relative to $\mathcal{G}^s$, The length of the orbit is the index $|\mathcal{G} : \mathcal{G}^s|$.
All members of an orbit have conjugate little groups: if $\mathcal{G}^s$ is the little group of $\mathbf{D}^{(s)}(\mathcal{H})$, then $\mathcal{G}^{(s)}_{g_i} = g_i \mathcal{G}^s g_i^{-1}$ is the little group of $(\mathbf{D}^{(s)}(\mathcal{H}))_{g_i}$.

Our aim is to develop an induction procedure for the construction of the irreps of $\mathcal{G}$, given the irreps $\mathbf{D}^{(s)}(\mathcal{H})$. For that it is necessary to consider the induction from the irreps of the little group $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H}))$. However, $\mathcal{G}^s$ may have many irreps. Only some of them are of interest for the derivation of the irreps of $\mathcal{G}$. These are the so-called *allowed* irreps (known also as *allowable irreps* or *small irreps*) according to the following definition.

Definition (D 2.5.1.6) An irrep $\mathbf{D}^{(j)}(\mathcal{G}^s) \equiv \mathbf{D}^{(j)}(\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H})))$ is called *allowed* if its subduction to the group $\mathcal{H}$ contains the irrep $\mathbf{D}^{(s)}(\mathcal{H})$ of $\mathcal{H}$.

Now one can state the theorem which permits the construction of the irreps of a group $\mathcal{G}$ provided the irreps of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ are known. One considers the groups $\mathcal{G}$ and $\mathcal{H}$ and the orbits $O(\mathbf{D}^{(j)}(\mathcal{H}))$ relative to $\mathcal{G}$.

Lemma 2.5.2 **Induction Theorem**

(a) Let $\mathbf{D}^{(j)}(\mathcal{H})$ be an irrep from the orbit $O(\mathbf{D}^{(j)}(\mathcal{H}))$ with the little group $\mathcal{G}^j(\mathbf{D}^{(j)}(\mathcal{H}))$ relative to $\mathcal{G}$. Then each allowed irrep $\mathbf{D}^{(m)}(\mathcal{G}^j(\mathbf{D}^{(j)}(\mathcal{H})))$ of $\mathcal{G}^j(\mathbf{D}^{(j)}(\mathcal{H}))$induces an irrep $\boldsymbol{D}^{Ind}(\mathcal{G})$, whose subduction to $\mathcal{H}$ yields the orbit $O(\mathbf{D}^{(j)}(\mathcal{H}))$.

(b) All irreps of $\mathcal{G}$ are obtained exactly once if the procedure described in (a) is applied on one irrep $\mathbf{D}^{(j)}(\mathcal{H})$ from each orbit $O(\mathbf{D}^{(j)}(\mathcal{H}))$ of irreps of $\mathcal{H}$ relative to $\mathcal{G}$.

By this theorem the problem of determining the irreps of a group $\mathcal{G}$ from those of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ is reduced to the determination of the allowed irreps of the little group $\mathcal{G}^j(\mathbf{D}^{(j)}(\mathcal{H}))$. For their determination one can use the theorem stated above and the fact that the crystallographic point groups $\mathcal{G}$ of 3-dimensional space are solvable groups (*cf.* Sections 1.5.2 and 1.5.3).

2.5.2 The special procedure for indices 2 and 3

If the group $\mathcal{H}$ is a normal subgroup of the group $\mathcal{G}$ of index 2 or index 3, then the little group $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H}))$ of any irrep of $\mathcal{H}$ is either the group $\mathcal{G}$ or its normal subgroup $\mathcal{H}$ because of the prime index. Two cases are to be distinguished:

1. The orbit has the length 2 or 3, $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H})) = \mathcal{H}$.

2. The orbit has the length 1, *i. e.* $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H})) = \mathcal{G}$.

Orbits of irreps of lengths 2 and 3

One can now make use of the obtained results for those cases where the length of the orbit is not trivial, *i. e.* where the orbit is not self-conjugate. For a normal subgroup of index 2 or 3 one can decompose $\mathcal{G}$ into cosets relative to $\mathcal{H}$, *i. e.* $\mathcal{G} = \mathcal{H} \cup q\mathcal{H}$ for index 2, and $\mathcal{G} = \mathcal{H} \cup q\mathcal{H} \cup q^2\mathcal{H}$ for index 3 with $q \in \mathcal{G}$ but $q \notin \mathcal{H}$.
The orbits of conjugate irreps have the form:

- index 2: $O(\mathbf{D}^{(s)}(\mathcal{H})) = \{\mathbf{D}^{(s)}(\mathcal{H}),\ (\mathbf{D}^{(s)}(\mathcal{H}))_q\}$
- index 3: $O(\mathbf{D}^{(s)}(\mathcal{H})) = \{\mathbf{D}^{(s)}(\mathcal{H}),\ (\mathbf{D}^{(s)}(\mathcal{H}))_q,\ (\mathbf{D}^{(s)}(\mathcal{H}))_{q^2}\}$.

In both cases there is just one allowed irrep which is the irrep $\mathbf{D}^{(s)}(\mathcal{H})$ itself, because $\mathcal{G}^s = \mathcal{H}$. An irrep of $\mathcal{G}$ can be induced from $\mathbf{D}^{(s)}(\mathcal{H})$ following the general induction procedure, see Section 2.5.1.

For example, for index 2 the auxiliary table necessary for the construction of the induced irrep has the form, *cf.* Section 2.5.1

g	g_i	$g_i^{-1}\,g$	g_j	$g_i^{-1}\,g\,g_j$	$M_{ij} \neq 0$
h	e	h	e	$e\,h\,e = h$	M_{11}
	q	$q^{-1}\,h$	q	$q^{-1}\,h\,q = (h)_q$	M_{22}
q	e	q	q	q^2	M_{12}
	q	$q^{-1}\,q = e$	e	e	M_{21}

which results in the following matrices for the induced rep $\mathbf{D}^{Ind}(\mathcal{G})$:

$$\mathbf{D}^{Ind}(h) = \begin{pmatrix} \boldsymbol{D}^{(s)}(h) & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_q \end{pmatrix};\ \mathbf{D}^{Ind}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{D}^{(s)}(q^2) \\ \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}. \tag{2.5.5}$$

Similarly, the general procedure reduces for index 3:

$$\mathbf{D}^{Ind}(h) = \begin{pmatrix} \boldsymbol{D}^{(s)}(h) & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_q & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_{q^2} \end{pmatrix}; \mathbf{D}^{Ind}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{D}^{(s)}(q^3) \\ \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}. \tag{2.5.6}$$

From the induction theorem on p. 37 follows that each orbit of conjugate irreps of $\mathcal{H}$ yields exactly one irrep of $\mathcal{G}$.

Self-conjugate irreps

If the length of the orbit is 1, *i. e.* the irrep of $\mathcal{H}$ is self-conjugate, then for the little group $\mathcal{G}^s = \mathcal{G}$ holds. The general theorem is now not very useful as the allowed irreps of the little groups are irreps of $\mathcal{G}$ which we want to determine. However, each self-conjugate irrep of $\mathcal{H}$ gives rise to $|\mathcal{G}/\mathcal{H}|$ irreps of $\mathcal{G}$ with the same dimension as $\mathbf{D}^{(s)}(\mathcal{H})$ has. The matrices of the irreps $\mathbf{D}^{(s),m}(\mathcal{G})$, $m = 1,\ 2$ or $m = 1,\ 2,\ 3$, derived from the self-conjugate irrep $\mathbf{D}^{(s)}(\mathcal{H})$, are given as follows:

index 2

$$\boldsymbol{D}^{(s),1}(h) = \boldsymbol{D}^{(s),2}(h) = \boldsymbol{D}^{(s)}(h),\ h \in \mathcal{H} \qquad \boldsymbol{D}^{(s),1}(q) = -\boldsymbol{D}^{(s),2}(q) = \boldsymbol{U} \tag{2.5.7}$$

where $\boldsymbol{U}$ is determined by the conditions

$$\boldsymbol{D}^{(s)}(q^{-1}\,h\,q) = \boldsymbol{U}^{-1}\,\boldsymbol{D}^{(s)}(h)\,\boldsymbol{U},\ h \in \mathcal{H}; \qquad \boldsymbol{U}^2 = \boldsymbol{D}^{(s)}(q^2)$$

index 3

$$\boldsymbol{D}^{(s),m}(h) = \boldsymbol{D}^{(s)}(h),\ m = 1,\ 2,\ 3 \qquad \boldsymbol{D}^{(s),1}(q) = \epsilon\boldsymbol{D}^{(s),2}(q) = \epsilon^2\boldsymbol{D}^{(s),3}(q) = \boldsymbol{U} \tag{2.5.8}$$

with $\epsilon = \exp 2\pi i/3$, where $\boldsymbol{U}$ is determined by the conditions

$$\boldsymbol{D}^{(s)}(q^{-1}\,h\,q) = \boldsymbol{U}^{-1}\,\boldsymbol{D}^{(s)}(h)\,\boldsymbol{U},\ h \in \mathcal{H} \ \text{ and } \ \boldsymbol{U}^3 = \boldsymbol{D}^{(s)}(q^3)$$

2.6 Exercises

2.6.1 General introduction to group representations

- **Exercise** 2.6.1.1. Faithful representation of *4mm*

  (a) Construct a two-dimensional faithful representation D of *4mm* starting from the matrices of its generators: $\mathbf{D}(4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ $\mathbf{D}(m_{100}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

  (b) Determine the matrices of the two-dimensional faithful representation D' of *4mm* with respect to the new basis $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ and $\mathbf{b}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$.

  (c) Show that the two representations D and D' of the group *4mm* determined in (a) and (b) are equivalent, *i. e.* show that there exists a matrix $\mathbf{X}$ such that $\mathbf{X}^{-1}\mathbf{D}(g)\mathbf{X} = \mathbf{D'}(g)$, with $g \in 4mm$.

  Hint: The determination of $\mathbf{X}$ such that $\mathbf{D'} = \mathbf{X}^{-1}\mathbf{D}\mathbf{X}$ is equivalent to determine $\mathbf{X}$ such that $\mathbf{X}\mathbf{D'} = \mathbf{D}\mathbf{X}$ with the additional condition that *det* $\mathbf{X} \neq 0$.

- **Exercise** 2.6.1.2. Irreps of the cyclic group C_4

  The cyclic group C_4 of order 4 is generated by the element $< g >$. Two of the following three representations of C_4 are equivalent:

  $$\mathbf{D}_1(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \quad \mathbf{D}_2(g) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \mathbf{D}_3(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

  Determine which of the two are equivalent and find the corresponding similarity matrix. Can you give an argument why the third representation is not equivalent?

- **Exercise** 2.6.1.3. Schur Lemma

  (i) Determine the general form of the matrix $\mathbf{B}$ that commutes with the matrices of all elements of the two-dimensional irrep E of *4mm*: $\mathbf{E}(g)\mathbf{B} = \mathbf{B}\mathbf{E}(g)$, $\quad g \in 4mm$ $(*)$, where

  $$\mathbf{E}(4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \text{ and } \mathbf{E}(m_{10}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

  Hint: To determine $\mathbf{B}$ it is sufficient to consider the commuting equations $(*)$ for the generators of $4mm$.

  (ii) Show that the irreps of Abelian groups are one-dimensional.

- **Exercise** 2.6.1.4. Number and dimensions of irreps

  1. Determine the number and dimensions of the irreps of group 222. Can you write down the irrep table of the group 222?
  2. Determine the number and dimensions of the irreps of the group $4mm$. What about the irreps of 422? And those of $4/mmm$?
  3. Determine the number and dimensions of the irreps of the group $3m$. What about the irreps of 32? And those of $\bar{3}m$?

- **Exercise** 2.6.1.5. Character tables of point-group irreps

  1. Determine the character table of the group $4mm$. What about the character table of 422?

2. Consider the character table of the group 432. Determine the characters of the two-dimensional irrep E.

432	$\mathit{1}\,(1)$	$\mathit{2}_{100}\,(3)$	$\mathit{2}_{110}\,(6)$	$\mathit{3}^{+}_{111}\,(8)$	$\mathit{4}^{+}_{100}\,(6)$
$\mathbf{A}_1$	1	1	1	1	1
$\mathbf{A}_2$	1	1	−1	1	−1
$\mathbf{E}$	?	?	?	?	?
$\mathbf{T}_1$	3	−1	−1	0	1
$\mathbf{T}_2$	3	−1	1	0	−1

- **Exercise** 2.6.1.6. Consider the group 222 and its irreps. Show that the following matrices form a representation of 222 that is reducible:

$$\mathbf{D}(e) = \mathbf{D}(2_{001}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \mathbf{D}(2_{100}) = \mathbf{D}(2_{010}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

1. Decompose the reducible representation into irreps of 222;
2. Calculate the matrix $\mathbf{S}$ that reduces the reducible representation D into irreducible constituents D_i: $\mathbf{D}(\mathcal{G})\mathbf{S} = \mathbf{S}[\oplus\mathbf{D}_i(\mathcal{G})]$.

- **Exercise** 2.6.1.7. Vector representation of *4mm*

1. Construct the vector representation of the point group *4mm* from the 'general position' of the space-group table of *P4mm* in *IT* A (*cf.* Fig. **??**, page **??**).
2. What is the difference between this vector representation and that can be obtained from the the space-group data of *P4bm* in *IT* A (*cf.* Fig. 4.2, page 56)?
3. Is the vector representation of point group *4mm* reducible or irreducible? Determine the general form of a matrix that commutes with all matrices of the vector representation of *4mm*.
4. If it is reducible, decompose it into irreducible constituents.

- **Exercise** 2.6.1.8. Consider the character table of the irreps of the group 422 and the following three reducible representations of the group specified by their characters:

$\psi_1(\mathit{e}) = 6$, $\psi_1(2_{100}) = 2$, $\psi_1(4) = \psi_1(2_{100}) = \psi_1(2_{110}) = 0$

$\psi_2(\mathit{e}) = 10$, $\psi_1(2_{100}) = 6$, $\psi_2(4) = \psi_1(2_{100}) = -2$ and $\psi_2(2_{110}) = 0$

$\psi_3(\mathit{e}) = 11$, $\psi_1(2_{100}) = 7$, $\psi_1(4) = \psi_1(2_{100}) = \psi_1(2_{110}) = -3$

Determine the decomposition of the reducible representations into irreps of 422.

2.6.2 Direct product of irreps and subduced representations

- **Exercise** 2.6.2.1. Kronecker product of matrices

Calculate the Kronecker products $\mathbf{A} \bigotimes \mathbf{B}$ and $\mathbf{B} \bigotimes \mathbf{A}$ of the following two matrices

$$\mathbf{A} = \begin{pmatrix} -1 & -2 \\ 1 & 2 \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} 1 & 1 & 2 \\ 1 & -1 & 1 \\ 0 & 2 & -1 \end{pmatrix}$$

What is the trace of the matrix $\mathbf{A} \bigotimes \mathbf{B}$? And of $\mathbf{B} \bigotimes \mathbf{A}$?

- **Exercise** 2.6.2.2. Irrep multiplication tables

    1. Construct the irrep multiplication table of the group $4mm$
    2. Construct the irrep multiplication table of the group $3m$

- **Exercise** 2.6.2.3. Symmetrized and anti-symmetrized irreps squares

    1. Calculate the characters of the symmetrized $\{E\}^2$ and antisymmetrized $[E]^2$ squares of the two dimensional irreps of $4mm$. If $\{E\}^2$ and/or $[E]^2$ are reducible, decompose them into irreps of $4mm$.
    2. The same for the two-dimensional irrep of the group $3m$.

- **Exercise** 2.6.2.4. Irreps of direct-product groups

    1. Determine the character table of the group $222 \cong 2 \times 2'$ from the character table of the cyclic groups 2.
    2. Determine the character table of the group $4/mmm \cong 422 \times \bar{1}$ starting from the character tables of the groups 422 and $\bar{1}$.
    3. Determine the character table of the group $4/m \cong 4 \times \bar{1}$ starting from the character tables of the cyclic groups 4 and $\bar{1}$.
    4. determine the character table of the group $6 \cong 3 \times 2$ from the character tables of the cyclic groups 3 and 2.

- **Exercise** 2.6.2.5.

    Consider the two-dimensional irrep $\mathbf{E}$ of point group *4mm* (see Problem 2.6.1.7 and Section 4.4.2) and its subgroup *4*.

    1. Is the subduced representation $\mathbf{E} \downarrow 4$ reducible or irreducible ?
    2. If reducible, decompose it into irreps of *4*.
    3. Determine the corresponding subduction matrix $\boldsymbol{S}$, defined by $\boldsymbol{S}^{-1}\,(\mathbf{E} \downarrow 4)(h)\,\boldsymbol{S} = \oplus m_i\,\mathbf{D}^i(h)$, $h \in$ *4*.

- **Exercise** 2.6.2.6.

    Consider the two-dimensional irrep $\mathbf{E}$ of point group *4mm* (see Problem 2.6.1.7 and Section 4.4.2) and its subgroup *mm2*.

    1. Is the subduced representation $\mathbf{E} \downarrow mm2$ reducible or irreducible ?
    2. If reducible, decompose it into irreps of *mm2*.
    3. Determine the corresponding subduction matrix $\boldsymbol{S}$, defined by $\boldsymbol{S}^{-1}\,(\mathbf{E} \downarrow mm2)(h)\,\boldsymbol{S} = \oplus m_i\,\mathbf{D}^i(h)$, $h \in$ *mm2*.

- **Exercise** 2.6.2.7.

    Construct the general form of the matrices of a representation of $\mathcal{G}$ induced by the irreps of a subgroup $\mathcal{H} < \mathcal{G}$ of index 2.

- **Exercise** 2.6.2.8.

    Construct the general form of the matrices of a representation of $\mathcal{G}$ induced by the irreps of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ of index 3.

- **Exercise** 2.6.2.9.

  Determine the representations of the group *4mm* induced from the irreps of its subgroup $\{1, m_{010}\}$ (for the necessary data see Sections 4.3 and 4.5). What are the dimensions of the induced representations of *4mm*? Are they reducible or irreducible?

- **Exercise** 2.6.2.10.

  Consider the two-dimensional irrep **E** of point group *4mm* (*cf.* Section 4.4.2):

  1. Is the direct-product representation $\mathbf{E} \otimes \mathbf{E}$ reducible or irreducible?
  2. If reducible, find its decomposition into irreps of *4mm*;
  3. If the functions $\{f_x, f_y\}$ form the basis of **E**, can you guess if it would be possible to construct invariants from the functions of the product carrier space $\{f_x^2, f_x f_y, f_y f_x, f_y^2\}$?
  4. If possible, how many invariants can be constructed, and what are the corresponding linear combinations of $f_i f_j$?

Chapter 3

Irreducible representations of space groups

For the derivation of all irreps of a space group we use the method of constructing the irreps of a group $\mathcal{G}$ from those of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ (can be demonstrated in a straightforward way by the derivation of the irreps of point groups). The main steps of the procedure are:

1. Construct all irreps of $\mathcal{H}$
2. Distribute the irreps of $\mathcal{H}$ into orbits under $\mathcal{G}$ and select one member of each orbit
3. Determine the little group for each selected irrep of $\mathcal{H}$
4. Find the allowed (small) irreps of the little group
5. The irreps of $\mathcal{G}$ are constructed from the allowed irreps of the little group by induction.

The set of all irreps of $\mathcal{G}$ is complete if the induction is applied to all allowed irreps of the little group for each selected irrep of $\mathcal{H}$.

The *translation group* $\mathcal{T}$ is a normal subgroup of every space group. The irreps of $\mathcal{T}$ and their distribution into orbits will be discussed in Section 3.1 and Section 3.2. The determination of the little groups of the selected irreps (step 3) and the induction procedure (step 5) are dealt with in Sections 3.2 and 3.4 The most involved step in the above procedure is the determination of the allowed irreps of the little group (step 4). In most books on irreps of space groups this difficulty is removed by applying the theory of the so-called *projective reps*. Here we have preferred another approach for the construction of the small irreps. It is based on the fact that all space groups are *solvable groups*, *i. e.* for every space group one can construct a *composition series*

$$\mathcal{G} \rhd \mathcal{H}_1 \rhd \mathcal{H}_2 \ \ldots \ \rhd \mathcal{T}$$

such that all factor groups $\mathcal{H}_i/\mathcal{H}_{i+1}$ are cyclic groups of order 2 or 3 (for details, *cf.* Section 1.5.2). For the space-group representation theory we follow the terminology of BC and CDML.

3.1 Representations of the translation group $\mathcal{T}$

Let $\mathcal{G}$ be referred to a primitive basis. The infinite set of translations $(\boldsymbol{I}, \boldsymbol{t})$, with $\boldsymbol{t}$ being the column of integers $(n_1,\ n_2,\ n_3)$ is based on discrete cyclic groups of infinite order. For the following, this group will

be replaced by a (very large) finite set in the usual way: One assumes the Born-von Karman boundary conditions

$$(\boldsymbol{I},\, \boldsymbol{t}_i)^{N_i} = (\boldsymbol{I},\, \boldsymbol{N}_i) = (\boldsymbol{I},\, \boldsymbol{o}) \tag{3.1.1}$$

to hold, where $\boldsymbol{t}_i$ = (1,0,0), (0,1,0), or (0,0,1) and N_i is a large integer for i = 1, 2, or 3, respectively. Then for any lattice translation ($\boldsymbol{I}$, $\boldsymbol{t}$)

$$(\boldsymbol{I},\, \boldsymbol{N}\boldsymbol{t}) = (\boldsymbol{I},\, \boldsymbol{o}) \qquad \text{holds,} \tag{3.1.2}$$

where $\boldsymbol{N}\boldsymbol{t}$ is the column $(N_1 n_1, N_2 n_2, N_3 n_3)^{\mathrm{T}}$ (here $(\ )^{\mathrm{T}}$ stands for transposed relative to rows). If the (infinitely many) translations mapped in this way onto ($\boldsymbol{I}$, $\boldsymbol{o}$) form a normal subgroup $\mathcal{T}_1$ of $\mathcal{G}$, then there exists a factor group $\mathcal{G}' = \mathcal{G}/\mathcal{T}_1$ of $\mathcal{G}$ relative to $\mathcal{T}_1$ with translation subgroup $\mathcal{T}' = \mathcal{T}/\mathcal{T}_1$ which is finite and is sometimes called the *finite space group*.

Only the irreducible representations (irreps) of these finite space groups will be considered. The definition of space-group type, symmorphic space group, *etc.* can be transferred to these groups. Because $\mathcal{T}$ is Abelian, $\mathcal{T}'$ is also Abelian. Replacing the space group $\mathcal{G}$ by $\mathcal{G}'$ means that the particularly well-developed theory of representations of finite groups can be applied. For convenience, the prime $'$ will be omitted and the symbol $\mathcal{G}$ will be used instead of $\mathcal{G}', \mathcal{T}'$ will be denoted by $\mathcal{T}$ in the following.

Because $\mathcal{T}$, *i.e.* former $\mathcal{T}'$, is Abelian, its irreps $\boldsymbol{\Gamma}(\mathcal{T})$ are one-dimensional and consist of (complex) roots of unity. Due to the equations (3.1.1) and (3.1.2) the irreps $\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\, \boldsymbol{t})]$ of $\mathcal{T}$ have the form

$$\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\, \boldsymbol{t})] = e^{-2\pi i (q_1 \frac{n_1}{N_1} + q_2 \frac{n_2}{N_2} + q_3 \frac{n_3}{N_3})}, \tag{3.1.3}$$

where n_k, q_j, = 0, 1, 2, $\ldots$, $N_j - 1$, $j = 1, 2, 3$, n_k, and q_j are integers.

Given a primitive basis $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ of $\mathbf{L}$, mathematicians and crystallographers define the *basis of the reciprocal lattice* $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ (or *basis of the dual lattice*) $\mathbf{L}^*$ by

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \tag{3.1.4}$$

where $\mathbf{a}\cdot\mathbf{a}^*$ means the scalar product between the vectors, and δ_{ij} is the unit matrix (see, *e.g.*, International Tables for Crystallography, Vol. B (2008), Subsection 1.1.3). Texts on physics of solids redefine the basis $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ of the *reciprocal lattice* $\mathbf{L}^*$, lengthening each of the basis vectors $\mathbf{a}_j^*$ by the factor 2π. Therefore, in the physicist's convention the relation between the bases of direct and reciprocal lattice reads, *cf.* BC, p. 86:

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}. \tag{3.1.5}$$

In the present chapter only the physicist's basis of the reciprocal lattice is employed, and hence the use of $\mathbf{a}_j^*$ should not lead to misunderstandings. The set of all vectors $\mathbf{K}$[1],

$$\mathbf{K} = K_1\mathbf{a}_1^* + K_2\mathbf{a}_2^* + K_3\mathbf{a}_3^*, \tag{3.1.6}$$

K_i integer, is called the lattice reciprocal to $\mathbf{L}$ or the *reciprocal lattice* $\mathbf{L}^*$ [2].
If one adopts the notation of *IT*A , the basis of direct space is denoted by a row $(\mathbf{a}_i)$=($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$). For the reciprocal space, the basis is described by a column $(\mathbf{a}_i^*)^{\mathrm{T}}$= $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*)^{\mathrm{T}}$.

[1] In crystallography vectors are designated by small bold-faced letters. With $\mathbf{K}$ we make an exception in order to follow the tradition of physics. A crystallographic alternative could be $\mathbf{t}^*$.

[2] The lattice $\mathbf{L}$ is often called the *direct lattice*. These names are historically introduced and cannot be changed anymore, although equations (3.1.4) and (3.1.5) show that essentially none of the lattices is preferred: they form a pair of *mutually reciprocal* lattices.

As is well known, the Bravais type of the reciprocal lattice $\mathbf{L}^*$ is not necessarily the same as that of its direct lattice $\mathbf{L}$. If $\boldsymbol{W}$ is the matrix of a (point-) symmetry operation of the direct lattice, referred to its basis $(\mathbf{a}_i)$, then $\boldsymbol{W}^{-1}$ is the matrix of the same symmetry operation of the reciprocal lattice but referred to the dual basis $(\mathbf{a}_i^*)^{\mathrm{T}}$. This does not affect the symmetry because in a (symmetry) group with each element its inverse also belongs to the group. Therefore, the (point) symmetries of a lattice and its reciprocal lattice are always the same. However, there may be differences in the matrix descriptions due to the different orientations of $\mathbf{L}$ and $\mathbf{L}^*$ relative to the symmetry elements of $\overline{\mathcal{G}}$ and due to the reference to the different bases $(\mathbf{a}_i)$ and $(\mathbf{a}_i^*)^{\mathrm{T}}$. For example, if $\mathbf{L}$ has the point symmetry (Hermann-Mauguin symbol) $\overline{3}m1$, then the symbol for the point symmetry of $\mathbf{L}^*$ is $\overline{3}1m$ and *vice versa*.

Let $(\mathbf{a}_i)$ be a conventional basis of the lattice $\mathbf{L}$ of the space group $\mathcal{G}$. With the relations (3.1.5), $k_i = q_i/N_i$, and $\mathbf{k} = \sum_{i=1}^{3} k_i \mathbf{a}_i^*$, equation (3.1.3) can be written

$$\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\boldsymbol{t})] = \boldsymbol{\Gamma}^{\mathbf{k}}[(\boldsymbol{I},\boldsymbol{t})] = \exp - i(\mathbf{k}\,\mathbf{t}). \tag{3.1.7}$$

Equation (3.1.7) has the same form if a primitive basis $(\mathbf{p}_i)$ of $\mathbf{L}$ has been chosen. In this case the vector $\mathbf{k}$ is given by $\mathbf{k} = \sum_{i=1}^{3} k_{pi}\,\mathbf{p}_i^*$.

Let a primitive basis $(\mathbf{p}_i)$ be chosen for the lattice $\mathbf{L}$. The set of all vectors $\mathbf{k}$ (known as wave vectors) forms a discontinuous array. Consider two wave vectors $\mathbf{k}$ and $\mathbf{k}' = \mathbf{k} + \mathbf{K}$, where $\mathbf{K}$ is a vector of the reciprocal lattice $\mathbf{L}^*$. Obviously $\mathbf{k}$ and $\mathbf{k}'$ describe the same irrep of $\mathcal{T}$. Therefore, to determine all irreps of $\mathcal{T}$ it is necessary to consider only the wave vectors of a small region of the reciprocal space, where the translation of this region by all vectors of $\mathbf{L}^*$ fills the reciprocal space without gap or overlap. Such a region is called a *fundamental region* of $\mathbf{L}^*$ (the nomenclature in literature is not quite uniform. We follow here widely adopted definitions).

The fundamental region of $\mathbf{L}^*$ is not uniquely determined. Two types of fundamental regions are of interest in this chapter:

1. the *first Brillouin zone* or simply *Brillouin zone*, abbreviated BZ, is that range of $\mathbf{k}$ space around $\mathbf{o}$ for which $|\,\mathbf{k}\,| \leq |\,\mathbf{K} - \mathbf{k}\,|$ holds for any vector $\mathbf{K} \in \mathbf{L}^*$ (*Wigner-Seitz cell* or *domain of influence* in $\mathbf{k}$ space). The Brillouin zone is used in books and articles on irreps of space groups;

2. the *crystallographic unit cell in reciprocal space*, for short: *unit cell*, is the set of all $\mathbf{k}$ vectors with $-1/2 < k_i \leq 1/2$. It corresponds to the unit cell used in crystallography for the description of crystal structures in direct space. However, the center is here the $\mathbf{o}$ vector.

3.2 Orbits of irreps of $\mathcal{T}$ and little groups

In the previous section the irreps of $\mathcal{T}$ have been determined. These irreps have now to be classified into orbits relative to $\mathcal{G}$.

By definition the orbit of an irrep $\boldsymbol{\Gamma}^{\mathbf{k}}(\mathcal{T})$ includes all non-equivalent irreps $\boldsymbol{\Gamma}^{\mathbf{k}'}(\mathcal{T})$ for which there exists a matrix-column pair $(\boldsymbol{W}, \boldsymbol{w})$ of $\boldsymbol{g} \in \mathcal{G}$ such that

$\boldsymbol{\Gamma}^{\mathbf{k}'}(\boldsymbol{I},\,\boldsymbol{t}) = \boldsymbol{\Gamma}^{\mathbf{k}}((\boldsymbol{W},\,\boldsymbol{w})^{-1}(\boldsymbol{I},\,\boldsymbol{t})(\boldsymbol{W},\,\boldsymbol{w}))$, $(\boldsymbol{I},\,\boldsymbol{t}) \in \mathcal{T}$.

From $(\boldsymbol{W},\boldsymbol{w})^{-1}\,(\boldsymbol{I},\boldsymbol{t})\,(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\,\boldsymbol{W}^{-1}\boldsymbol{t})$ follows
$\boldsymbol{\Gamma}^{\mathbf{k}'}(\boldsymbol{I},\boldsymbol{t}) = \boldsymbol{\Gamma}^{\mathbf{k}}(\boldsymbol{I},\,\boldsymbol{W}^{-1}\boldsymbol{t}) = \exp -(i\,\mathbf{k}\,(\boldsymbol{W}^{-1}\,\mathbf{t})) = \exp(-i\,(\mathbf{k}\,\boldsymbol{W}^{-1})\,\mathbf{t})$. Thus,

$$\mathbf{k}' = \mathbf{k}\,\boldsymbol{W}^{-1} + \mathbf{K}, \quad \mathbf{K} \in\ \mathbf{L}^* \tag{3.2.8}$$

By the lattice vector $\mathbf{K} \in \mathbf{L}^*$ the vector $\mathbf{k}'$ is brought back to the fundamental region in case it would be outside otherwise.

Let $\mathbf{k}$ be some $\mathbf{k}$ vector and $\boldsymbol{W}$ be the matrices of $\overline{\mathcal{G}}$.

Definition (D 3.2.0.1) The set of all matrices $\boldsymbol{W} \in \overline{\mathcal{G}}$ which leave the vector $\mathbf{k}$ invariant or change it to an equivalent one, *i. e.*

$$\mathbf{k} = \mathbf{k}\,\boldsymbol{W} + \mathbf{K}, \quad \mathbf{K} \in \mathbf{L}^*, \tag{3.2.9}$$

forms a group which is called the *little co-group* $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. The vector $\mathbf{k}$ is called a *general* $\mathbf{k}$ *vector* if $\overline{\mathcal{G}}^{\mathbf{k}} = \{\mathcal{I}\}$; otherwise $\overline{\mathcal{G}}^{\mathbf{k}} > \{\mathcal{I}\}$, and $\mathbf{k}$ is called a *special* $\mathbf{k}$ *vector*.

The little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ is a subgroup of the point group $\overline{\mathcal{G}}$. Consider the coset decomposition of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.

Definition (D 3.2.0.2) If $\{\boldsymbol{W}_m\}$ is a set of coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$, then the set $\star(\mathbf{k}) = \{\mathbf{k}\,\boldsymbol{W}_m + \mathbf{K}\}$ is called the *star of* $\mathbf{k}$ and the vectors $\mathbf{k}\,\boldsymbol{W}_m + \mathbf{K}$ are called the *arms of the star*.

Here again the lattice vector $\mathbf{K}$ is necessary if $\mathbf{k}\,\boldsymbol{W}_m$ is outside the fundamental region.

An orbit of $\boldsymbol{\Gamma}^{\mathbf{k}}(\mathcal{T})$ relative to $\mathcal{G}$ comprises all irreps $\boldsymbol{\Gamma}^{\mathbf{k}'}(\mathcal{T})$ with $\mathbf{k}'$ belonging to $\star\mathbf{k}$. From the classification of all $\mathbf{k}$ vectors into stars follows the distribution of the irreps of $\mathcal{T}$ into orbits relative to $\mathcal{G}$. The length of an orbit $O(\boldsymbol{\Gamma}^{\mathbf{k}}(\mathcal{T}))$ is equal to the number of arms of $\star\mathbf{k}$ which is the index of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$ in the point group $\overline{\mathcal{G}}$.

If $\mathbf{k}$ is general, then there are $|\overline{\mathcal{G}}|$ vectors (arms) from the star of $\mathbf{k}$ in each fundamental region. If $\mathbf{k}$ is special with little co-group $\overline{\mathcal{G}}^{\mathbf{k}} \geq \{\mathcal{I}\}$, then the number of arms of the star of $\mathbf{k}$ in the fundamental region is $|\overline{\mathcal{G}}|/|\overline{\mathcal{G}}^{\mathbf{k}}|$.

According to the induction theorem, lemma 2.5.1, in order to obtain each irrep of $\mathcal{G}$ exactly once, one needs one $\mathbf{k}$ vector per star. A simply connected part of the fundamental region which contains exactly one $\mathbf{k}$ vector of each star of $\mathbf{k}$, is called a *representation domain* $\boldsymbol{\Phi}$. Thus, for the determination of all irreps of $\mathcal{G}$ it is sufficient to consider the $\mathbf{k}$ vectors belonging to the representation domain.

We are now in the position to define the little group $\mathcal{G}^{\mathbf{k}}$ if the space group $\mathcal{G}$, its translation subgroup $\mathcal{T}$, and an irrep $\boldsymbol{\Gamma}^{\mathbf{k}}(\mathcal{T})$ are given. The little group is a space group and consists of all those elements of $\mathcal{G}$ whose rotation parts $\boldsymbol{W}$ leave either $\mathbf{k}$ unchanged or invert it into an equivalent vector.

Definition (D 3.2.0.3) The group of all elements $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$ for which $\boldsymbol{W} \in \overline{\mathcal{G}}^{\mathbf{k}}$, is called the *little group* $\mathcal{G}^{\mathbf{k}}$ *of* $\mathbf{k}$.

3.3 Allowed irreps of the little group

The irreps of space groups are obtained by induction from the allowed irreps of the little groups $\mathcal{G}^{\mathbf{k}}$ of $\mathbf{k}$. If $\mathbf{D}^{\mathbf{k},i}(\mathcal{G}^{\mathbf{k}})$ is an allowed irrep of $\mathcal{G}^{\mathbf{k}}$, then $\mathbf{D}^{\mathbf{k},i}(\boldsymbol{I}, \boldsymbol{t}) = \exp(-i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}$ holds. The matrix $\boldsymbol{I}$ is the identity matrix with $\dim(\boldsymbol{I}) = \dim(\mathbf{D}^{\mathbf{k},i}(\mathcal{G}^{\mathbf{k}}))$.

The determination of the allowed irreps is trivial for a $\mathbf{k}$ *vector in general position*. Then its star contains $|\overline{\mathcal{G}}|$ arms, *i. e.* its little group is the translation group. For a given $\mathbf{k}$ vector it has just one allowed irrep, namely the one which belongs to the $\mathbf{k}$ vector considered. Thus, every star in a general position contributes exactly one irrep of $\mathcal{G}$.

Under certain conditions one can express the allowed irreps of $\mathcal{G}^{\mathbf{k}}$ in terms of the irreps $\overline{\mathsf{D}}^{\mathbf{k},i}$ of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ for a *special* $\mathbf{k}$ *vector*.

Lemma 3.3.1 Let one of the following two conditions be satisfied

1. $\mathbf{k}$ is a vector of the interior of the BZ
2. $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group.

Then the number of non-equivalent allowed irreps $\mathsf{D}^{\mathbf{k},i}$ of the little group $\mathcal{G}^{\mathbf{k}}$ is the same as the number of non-equivalent irreps $\overline{\mathsf{D}}^{\mathbf{k},i}$ of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$, and their matrices are of the form:

$$\boldsymbol{D}^{\mathbf{k},i}(\boldsymbol{W},\boldsymbol{w}) = \exp -(i\,\mathbf{k}\,\mathbf{w})\,\overline{\boldsymbol{D}}^{\mathbf{k},i}(\boldsymbol{W}),\ \ (\boldsymbol{W},\boldsymbol{w}) \in \mathcal{G}^{\mathbf{k}}.$$

In this way the allowed irreps of $\mathcal{G}^{\mathbf{k}}$ are expressed by irreps of the point groups. Only certain stars on the surface of the BZ give rise to difficulties for non-symmorphic space groups. These cases can be solved by the method of deducing all irreps of a group $\mathcal{G}$ from the irreps of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ with index 2 or 3. Since the little groups are space groups and thus solvable groups, one can construct for them composition series with factor groups of order 2 or 3. The irreps of any non-symmorphic space group can be constructed step by step following the chain of normal subgroups, starting from the irreps of that symmorphic subgroup $\mathcal{H}_0$ of $\mathcal{G}$ which has the smallest index. For each space group there is always at least one symmorphic subgroup in the composition series from $\mathcal{T}$ to $\mathcal{G}$: its translation subgroup $\mathcal{T}$.

Only the allowed irreps of the little group $\mathcal{G}^{\mathbf{k}}$ are necessary for the construction of the irreps of $\mathcal{G}$. However, it is straightforward to show that the allowed irreps of a symmorphic subgroup $\mathcal{H}_0^{\mathbf{k}} < \mathcal{G}^{\mathbf{k}}$ yield allowed irreps of $\mathcal{G}^{\mathbf{k}}$. On the other hand, non-allowed irreps of $\mathcal{H}_0^{\mathbf{k}} < \mathcal{G}^{\mathbf{k}}$ yield non-allowed irreps of $\mathcal{G}^{\mathbf{k}}$. In other words, in order to obtain all allowed irreps of $\mathcal{G}^{\mathbf{k}}$ it is only necessary to consider the allowed irreps of the symmorphic subgroup $\mathcal{H}_0^{\mathbf{k}}$.

Consider a group-subgroup chain $\mathcal{G}^{\mathbf{k}} \rhd \mathcal{H}_0^{\mathbf{k}}$ with index 2 or 3. The irreps of $\mathcal{G}^{\mathbf{k}}$ are obtained from those of $\mathcal{H}_0^{\mathbf{k}}$ by the formulae discussed in Section 2.5.2. The allowed irreps of $\mathcal{H}_0^{\mathbf{k}}$ are those whose matrices of the translation elements are of the form:

$$\mathsf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}(\boldsymbol{I},\boldsymbol{t}) = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}. \tag{3.3.10}$$

For self-conjugate irreps allowed irreps of $\mathcal{H}_0^{\mathbf{k}}$ yield allowed irreps of $\mathcal{G}^{\mathbf{k}}$, see equation 2.5.7 and 2.5.8.

For induction from non-self-conjugate irreps of $\mathcal{H}_0^{\mathbf{k}}$, see equations 2.5.5 and 2.5.6, the above result is also valid

$$(\mathsf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}(\boldsymbol{I},\boldsymbol{t}))_{(\boldsymbol{W},\boldsymbol{w})} = \mathsf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}[(\boldsymbol{W},\boldsymbol{w})^{-1}(\boldsymbol{I},\boldsymbol{t})(\boldsymbol{W},\boldsymbol{w})] = \exp -(i\,(\mathbf{k}\,\boldsymbol{W}^{-1}\,\mathbf{t}))\,\boldsymbol{I} = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}, \tag{3.3.11}$$

because the coset representative $(\boldsymbol{W},\boldsymbol{w})$ of $\mathcal{G}^{\mathbf{k}}$ relative to $\mathcal{H}_0^{\mathbf{k}}$ leaves the $\mathbf{k}$ vector invariant (up to a lattice vector $\mathbf{K} \in \mathbf{L}^*$). From the discussion is also clear that non-allowed irreps of $\mathcal{H}_0^{\mathbf{k}}$ give rise to non-allowed irreps of $\mathcal{G}^{\mathbf{k}}$.

3.4 Induction procedure

All irreps of a space group $\mathcal{G}$ are obtained by taking a vector $\mathbf{k}$ from each star and inducing irreps of $\mathcal{G}$ from all non-equivalent allowed irreps $\mathsf{D}^{\mathbf{k},i}$ of the corresponding little group $\mathcal{G}^{\mathbf{k}}$. If $\dim(\mathsf{D}^{\mathbf{k},i}) = r$ and

s is the order of the star of $\mathbf{k}$, then the induced irrep $\mathbf{D}^{*\mathbf{k},i}(\mathcal{G})$ has the dimension $r\,s$. The matrices of $\mathbf{D}^{*\mathbf{k},i}(\mathcal{G})$ can be arranged in blocks $M_{i\,j}$ of dimension r, with one non-zero block in each row or column of blocks.

If we choose the elements $(\boldsymbol{W}_i,\,\boldsymbol{w}_i),\quad i=1,\,\ldots\,,s$ as representatives of the cosets of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$: $\mathcal{G}=\mathcal{G}^{\mathbf{k}}\cup(\boldsymbol{W}_2,\,\boldsymbol{w}_2)\,\mathcal{G}^{\mathbf{k}}\cup\,\ldots\,\cup(\boldsymbol{W}_s,\,\boldsymbol{w}_s)\,\mathcal{G}^{\mathbf{k}}$,

then the block $i\,j$ is zero unless $(\boldsymbol{W}_i,\,\boldsymbol{w}_i)^{-1}\,(\boldsymbol{W},\,\boldsymbol{w})\,(\boldsymbol{W}_j,\,\boldsymbol{w}_j)\in\mathcal{G}^{\mathbf{k}}$.

As was already discussed in Section 3.3, the little group $\mathcal{G}^{\mathbf{k}}$ of $\mathbf{k}$ is the translation group $\mathcal{T}$ if $\mathbf{k}$ is a vector of general position. Then $\mathbf{\Gamma}^{\mathbf{k}}(\mathcal{T})$ is the only allowed irrep.

The corresponding induced irrep of $\mathcal{G}$ has a dimension equal to the length of the orbit $*\mathbf{k}=\{\mathbf{k}_1,\,\mathbf{k}_2,\,\ldots,\,\mathbf{k}_n\}$, where $\mathbf{k}_i=\mathbf{k}\;\boldsymbol{W}_i+\mathbf{K}$ with $\boldsymbol{W}_i\in\overline{G}$.

The representation matrices corresponding to the elements of $\mathcal{T}$ are diagonal matrices, where the elements are the irreps of $\mathcal{T}$ belonging to the orbit of $\mathbf{k}$.

The representation matrices for any element of $\mathcal{G}$ and arbitrary $\mathbf{k}$ vector are obtained by the general induction method, see Section 2.5.1. For better efficiency it is advisable to calculate the non-zero blocks of the induction matrix first. Very often, for a better overview of the irreps of $\mathcal{G}$, their matrices are presented by the non-zero blocks of the induction matrix and the corresponding submatrices of the little-group irreps.

3.5 Exercises

3.5.1 Irreducible representations of space groups

- **Exercise** 3.5.1.1. Irreducible representations of the group *P4mm*(99)

  Consider the $\mathbf{k}$-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{X}\;(0\tfrac{1}{2}0)$ of the group *P4mm*.

  1. Determine the little groups, the $\mathbf{k}$-vector stars, the number and the dimensions of the allowed little-group irreps, the number and the dimensions of the corresponding full irreps of the group *P4mm*. Construct the allowed little group irreps of *P4mm* for $\mathbf{\Gamma}(000)$ and $\mathbf{X}(0\tfrac{1}{2}0)$;
  2. Calculate a set of coset representatives of the decomposition of the group *P4mm* with respect to the little groups of the $\mathbf{k}$-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{X}(0\tfrac{1}{2}0)$, and construct the corresponding full space group irreps of *P4mm*.

- **Exercise** 3.5.1.2. Irreducible representations of the group *P4bm*(100)

  Consider the $\mathbf{k}$-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{X}(0\tfrac{1}{2}0)$ of the group *P4bm*.

  1. Determine the irreps of space group *P4bm*, $\mathbf{k}=\mathbf{\Gamma}(000)$. Is there a difference to the irreps of space group *P4mm*, $\mathbf{k}=\mathbf{\Gamma}(000)$?
  2. Determine the allowed little-group irreps of space group *P4bm* for $\mathbf{k}$=$\mathbf{X}\;(0\tfrac{1}{2}0)$. Compare the obtained irreps with those obtained in the exercise with *P4mm*, $\mathbf{k}=\mathbf{X}(0\tfrac{1}{2}0)$.

- **Exercise** 3.5.1.3. Space-group irreps for a general $\mathbf{k}$-vector

  Consider a general $\mathbf{k}$-vector of a space group $\mathcal{G}$. Determine its little co-group, the $\mathbf{k}$-vector star. How many arms has its star? How many full-group irreps will be induced and of what dimension? Write down the matrix of the full-group irrep of a general $\mathbf{k}$-vector for a translation, $t\in\mathcal{T}_{\mathcal{G}}$.

- **Exercise** 3.5.1.4. Irreducible representations of the group $P2_13$ (198)

  Consider the $\mathbf{k}$-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{k}=\mathbf{R}(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})$ of the group $P2_13$.

1. Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group $P2_13$. Construct the little group irreps of $P2_13$ for $\mathbf{\Gamma}(000)$ and $\mathbf{k} = \mathbf{R}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$;
2. Calculate a set of coset representatives of the decomposition of the group $P2_13$ with respect to the little groups of the **k**-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{k} = \mathbf{R}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, and construct the corresponding full space group irreps of $P2_13$.

3.5.2 Tools of the Bilbao Crystallographic Server for Space-group Irreps

- **Exercise** 3.5.2.1.

  1. Obtain the irreps for the space group $P4mm(99)$ for the **k**-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{X}(0\frac{1}{2}0)$ using the program `REPRES`. Compare the results with the solutions of Problem 3.5.1.1.
  2. Use the program `REPRES` for the derivation of the irreps of a general **k**-vector of the group $P4mm$ and compare the results with the results of Problem 3.5.1.3.
  3. Use the program `Representations SG` for the derivation of the irreps for the **k**-vectors $\mathbf{\Gamma}(000)$, $\mathbf{X}(0\frac{1}{2}0)$ and of a general **k**-vector of the group $P4mm$ and compare the results with the results of Problems 3.5.1.1 and 3.5.1.3.

- **Exercise** 3.5.2.2.

  1. Obtain the irreps for the space group $P4bm(100)$ for the **k**-vectors $\mathbf{\Gamma}(000)$ and $\mathbf{X}(0\frac{1}{2}0)$ using the program `REPRES`. Compare the results with the solutions of Problem 3.5.1.2.
  2. Use the program `REPRES` for the derivation of the irreps of a general **k**-vector of the group $P4bm$ and compare the results with the results of Problem 3.5.1.3.
  3. Use the program `Representations SG` for the derivation of the irreps for the **k**-vectors $\mathbf{\Gamma}(000)$, $\mathbf{X}(0\frac{1}{2}0)$ and of a general **k**-vector of the group $P4mm$ and compare the results with the results of Problems 3.5.1.2 and 3.5.1.3.

- **Exercise** 3.5.2.3.

  The star of the wave vector $\mathbf{X}(\frac{1}{2}00)$ in the cubic group $Pm\text{-}3m(221)$ consists of three arms: ${}^*\mathbf{X} = \{(\frac{1}{2}00), (0\frac{1}{2}0), (00\frac{1}{2})\}$

  (i) Determine the wave-vector correlations (splttings) of **k**-vector star ${}^*\mathbf{X}$ for the group-subgroup chain $Pm\bar{3}m(\mathbf{a},\mathbf{b},\mathbf{c}) > P4mm(\mathbf{a},\mathbf{b},\mathbf{c})$

  (ii) How the wave-vector correlations of ${}^*\mathbf{X}$ change if unit cell of the low-symmetry group is doubled along c axis, *i. e.* the group-subgroup chain is of the type $Pm\bar{3}m(\mathbf{a},\mathbf{b},\mathbf{c}) > P4mm(\mathbf{a},\mathbf{b},2\mathbf{c})$

  (iii) Compare your results with the output of the program `CORREL` .

- **Exercise** 3.5.2.4.

  Using the program `COMPATIBILITY RELATIONS` determine the connectivity of the electronic energy bands of Ge, symmetry group $Fd\bar{3}m(227)$, between the high symmetry points $\mathbf{\Gamma}(000)$ and $\mathbf{X}(\frac{1}{2}0\frac{1}{2})$ over the symmetry line $\mathbf{\Delta}(u0u)$ (*cf.* BZ data of $Fd\bar{3}m$ provided by the program `KVEC`).

- **Exercise** 3.5.2.5.

  (a) Consider the space group $P4mm$ and its **k**-vector $\mathbf{X}(0\frac{1}{2}0)$. Determine the wave-vector selection rules for the product of the **k**-vector stars: ${}^*\mathbf{X}(0\frac{1}{2}0) \otimes {}^*\mathbf{X}(0\frac{1}{2}0)$.

  (b) Consider the space group $P4/mmm$(No. 123) and its **k**-vector $\mathbf{X}(0\frac{1}{2}0)$ and $\mathbf{\Delta}(0, 0.27, 0)$. Determine the wave-vector selection rules for the product ${}^*\mathbf{\Delta}(0, 0.27, 0) \otimes {}^*\mathbf{X}(0\frac{1}{2}0)$.

  (c) Compare your results with the output of the program `DIRPRO` .

Chapter 4

Appendix

The Appendix contains the procedures and necessary basic data for the exercises: multiplication tables, matrices, character tables, *etc.*

4.1 Procedure for the construction of the irreps of space groups.

The main steps for constructing the irreps of space groups can be summarized as follows

1. Space-group information
   (a) Decomposition of the space group $\mathcal{G}$ in cosets relative to its translation subgroup $\mathcal{T}$, see IT A (1996)
   $\mathcal{G} = \mathcal{T} \cup (\boldsymbol{W}_2,\, \boldsymbol{w}_2)\,\mathcal{T} \cup \ \ldots\ \cup (\boldsymbol{W}_p,\, \boldsymbol{w}_p)\,\mathcal{T}$
   (b) Choice of a convenient set of generators of $\mathcal{G}$, see IT A (1996)
2. **k**-vector information
   (a) Choice of a **k** vector (from the rep domain $\boldsymbol{\Phi}$ of the BZ). The coefficients of the **k** vector have to be referred to the dual basis of that basis relative to which the space group is defined:
   (b) Determination of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of **k**:
   $\overline{\mathcal{G}}^{\mathbf{k}} = \{\,\widetilde{\boldsymbol{W}}_i \in \overline{\mathcal{G}} :\ \boldsymbol{k} = \boldsymbol{k}\,\widetilde{\boldsymbol{W}}_i + \boldsymbol{K},\ \mathbf{K} \in \mathbf{L}^*\}$
   (c) Determination of the **k**-vector star $\star(\mathbf{k})$
   $\star(\mathbf{k}) = \{\mathbf{k},\ \mathbf{k}_2,\ \ldots\ , \mathbf{k}_s\}$, with $\mathbf{k} = \mathbf{k}\,\overline{\boldsymbol{W}}_j,\ j = 1,\ \ldots\ s$, where $\overline{W}_j$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.
   (d) Determination of the little group $\mathcal{G}^{\mathbf{k}}$
   $\mathcal{G}^{\mathbf{k}} = \{(\widetilde{\boldsymbol{W}}_i,\, \widetilde{\boldsymbol{w}}_i) \in \mathcal{G} :\ \widetilde{\boldsymbol{W}}_i \in \overline{\mathcal{G}}^{\mathbf{k}}\}$
   (e) Decomposition of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$
   An obvious choice of coset representatives of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$ is the set of elements $\{q_i = (\overline{W}_i,\, \overline{w}_i),\, i = 1,\ \ldots,\ s\}$
   where $\overline{W}_i$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$
   $\mathcal{G} = \mathcal{G}^{\mathbf{k}} \cup (\overline{W}_2,\, \overline{w}_2)\,\mathcal{G}^{\mathbf{k}} \cup \ \ldots\ (\overline{W}_s,\, \overline{w}_s)\,\mathcal{G}^{\mathbf{k}}$
3. Allowed irreps of $\mathcal{G}^{\mathbf{k}}$

(a) If $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group or $\mathbf{k}$ is inside the BZ, then the non-equivalent allowed irreps $\mathsf{D}^{\mathbf{k},i}$ of $\mathcal{G}^{\mathbf{k}}$ are related to the non-equivalent irreps $\overline{\mathsf{D}}^{\mathbf{k},i}$ of $\overline{\mathcal{G}}^{\mathbf{k}}$ in the following way: $\mathsf{D}^{\mathbf{k},i}(\widetilde{\boldsymbol{W}}_i,\, \widetilde{\boldsymbol{w}}_i) = \exp -(i\,\mathbf{k}\,\mathbf{w}_i)\,\overline{\mathsf{D}}^{\mathbf{k},i}(\widetilde{\boldsymbol{W}}_i)$

(b) If $\mathcal{G}^{\mathbf{k}}$ is a non-symmorphic space group and $\mathbf{k}$ is on the surface of the BZ, then:

i. Look for a symmorphic subgroup $\mathcal{H}_0^{\mathbf{k}}$ (or an appropriate chain of normal subgroups) of index 2 or 3

ii. Find the allowed irreps $\mathsf{D}^{\mathbf{k},i}_{\mathcal{H}_0}$ of $\mathcal{H}_0^{\mathbf{k}}$, *i. e.* those for which is fulfilled $\mathsf{D}^{\mathbf{k},i}_{\mathcal{H}_0}(\boldsymbol{I},\, \boldsymbol{t}) = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}$ and distribute them into orbits relative to $\mathcal{G}^{\mathbf{k}}$

iii. Determine the allowed irreps of $\mathcal{G}^{\mathbf{k}}$ using the results for the induction from the irreps of normal subgroups of index 2 or 3

4. Induction procedure for the construction of the irreps $\mathsf{D}^{\star\mathbf{k},i}$ of $\mathcal{G}$ from the allowed irreps $\mathsf{D}^{\mathbf{k},i}$ of $\mathcal{G}$
The representation matrices of $\mathsf{D}^{\star\mathbf{k},i}(\mathcal{G})$ for any element of $\mathcal{G}$ can be obtained if the matrices for the generators $\{(\boldsymbol{W}_l,\, \boldsymbol{w}_l),\ l = 1,\ \ldots, k\}$ of $\mathcal{G}$ are available (step 1a).

(a) Construction of the induction matrix.
The elements of the little group $\mathcal{G}^{\mathbf{k}} = \{(\widetilde{\boldsymbol{W}}_j,\, \widetilde{\boldsymbol{w}}_j)\}$ (step 2d) and the coset representatives $\{q_1, \ldots, q_s\}$ of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$ (step 2e) are necessary for the construction of the matrix $\boldsymbol{M}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$

$(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$	$q_i^{-1}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)q_j$	$M(\boldsymbol{W}_l,\, \boldsymbol{w}_l)_{ij} \neq 0$
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	

(b) Matrices of the irreps $\mathsf{D}^{\star\mathbf{k},m}$ of $\mathcal{G}$:

$\mathsf{D}^{\star\mathbf{k},m}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)_{i\mu,\,j\nu} = M(\boldsymbol{W}_l,\, \boldsymbol{w}_l)_{ij}\,\mathsf{D}^{\mathbf{k},m}(\widetilde{\boldsymbol{W}}_p,\, \widetilde{\boldsymbol{w}}_p)_{\mu\,\nu}$,

where $(\widetilde{\boldsymbol{W}}_p,\, \widetilde{\boldsymbol{w}}_p) = q_i^{-1}\,(\boldsymbol{W}_l,\, \boldsymbol{w}_l)\,q_j$.

All irreps of the space group $\mathcal{G}$ for a given $\mathbf{k}$ vector are obtained considering all allowed irreps $\mathsf{D}^{\mathbf{k},m}$ of the little group $\mathcal{G}^{\mathbf{k}}$ obtained in step 3.

4.2 Induction procedure for the case of normal subgroups of index 2 or 3

Start from the irreps D^s of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$, where $|\mathcal{G}/\mathcal{H}| = 2$ or 3.

1. Characterize the group-subgroup chain $\mathcal{G} \rhd \mathcal{H}$ by

(a) choice of appropriate generators for $\mathcal{H}$ and $\mathcal{G}$

(b) decompose $\mathcal{G}$ into cosets relative to $\mathcal{H}$ with coset representative q: $\mathsf{q} \in \mathcal{G}$ but $\mathsf{q} \notin \mathcal{H}$

i. $\mathcal{G} = \mathcal{H} \cup \mathsf{q}\,\mathcal{H}$ for index 2

ii. $\mathcal{G} = \mathcal{H} \cup \mathsf{q}\,\mathcal{H} \cup \mathsf{q}^2\,\mathcal{H}$ for index 3.

2. Determine the orbits of irreps of $\mathcal{H}$ relative to $\mathcal{G}$

- index 2:
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}) = (\mathbf{D}^s(\mathcal{H}))_q\}$ (self-conjugate)
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}),\, (\mathbf{D}^s(\mathcal{H}))_q\}$
- index 3:
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}) = (\mathbf{D}^s(\mathcal{H}))_q = (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$ (self-conjugate)
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}),\, (\mathbf{D}^s(\mathcal{H}))_q,\, (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$

3. Construct the irreps of $\mathcal{G}$

- index 2
  - $\{\mathbf{D}^s(\mathcal{H})\}$

$$\boldsymbol{D}^1(h) = \boldsymbol{D}^2(h) = \boldsymbol{D}^s(h),\ h \in \mathcal{H} \qquad \boldsymbol{D}^1(q) = -\boldsymbol{D}^2(q) = \boldsymbol{U}$$

    where $\boldsymbol{U}$ is determined by the conditions

$$\boldsymbol{D}^s(q^{-1}\, h\, q) = \boldsymbol{U}^{-1}\, \boldsymbol{D}^s(h)\, \boldsymbol{U},\ h \in \mathcal{H}; \qquad \boldsymbol{U}^2 = \boldsymbol{D}^s(q^2)$$

  - $\{\mathbf{D}^s(\mathcal{H}),\, (\mathbf{D}^s(\mathcal{H}))_q\}$

$$\mathbf{D}(h) = \begin{pmatrix} \boldsymbol{D}^s(h) & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^s(h))_q \end{pmatrix}; \mathbf{D}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{D}^s(q^2) \\ \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}.$$

- index 3
  - $\{\mathbf{D}^s(\mathcal{H})\}$

$$\boldsymbol{D}^m(h) = \boldsymbol{D}^s(h),\ m = 1,\ 2,\ 3 \qquad \boldsymbol{D}^m(q) = \omega^m\, \boldsymbol{U}$$

    where $\boldsymbol{U}$ is determined by the conditions

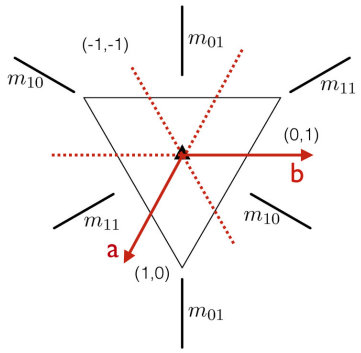
$$\boldsymbol{D}^s(q^{-1}\, h\, q) = \boldsymbol{U}^{-1}\, \boldsymbol{D}^s(h)\, \boldsymbol{U},\ h \in \mathcal{H}; \qquad \omega^3\, \boldsymbol{U}^3 = \boldsymbol{D}^s(q^3)$$

  - $\{\mathbf{D}^s(\mathcal{H}),\, (\mathbf{D}^s(\mathcal{H}))_q,\, (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$

$$\mathbf{D}(h) = \begin{pmatrix} \boldsymbol{D}^s(h) & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^s(h))_q & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & (\boldsymbol{D}^s(h))_{q^2} \end{pmatrix}; \quad \mathbf{D}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{D}^s(q^3) \\ \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}.$$

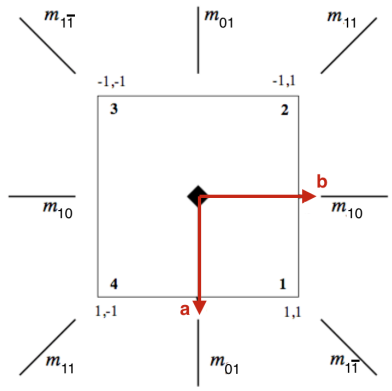
4.3 Multiplication (Cayley) tables

4.3.1 Symmetry elements and multiplication table of the group *3m*



$3m$	1	3^+	3^-	m_{11}	m_{10}	m_{01}
1	1	3^+	3^-	m_{11}	m_{10}	m_{01}
3^+	3^+	3^-	1	m_{01}	m_{11}	m_{10}
3^-	3^-	1	3^+	m_{10}	m_{01}	m_{11}
m_{11}	m_{11}	m_{10}	m_{01}	1	3^+	3^-
m_{10}	m_{10}	m_{01}	m_{11}	3^-	1	3^+
m_{01}	m_{01}	m_{11}	m_{10}	3^+	3^-	1

4.3.2 Symmetry elements and multiplication table of the group *4mm*



$4mm$	1	2	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
1	1	2	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
2	2	1	4^-	4^+	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
4^+	4^+	4^-	2	1	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
4^-	4^-	4^+	1	2	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	1	2	4^-	4^+
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	2	1	4^+	4^-
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^+	4^-	1	2
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^-	4^+	2	1

4.4 Matrix groups; generating matrices

4.4.1 Matrices of the group *3m*

$$\boldsymbol{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \boldsymbol{3}^+ = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}; \; \boldsymbol{3}^- = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix};$$

$$\boldsymbol{m}_{11} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}; \boldsymbol{m}_{10} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}; \boldsymbol{m}_{01} = \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix};$$

4.4.2 Matrices of the group *4mm*

$$\boldsymbol{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \boldsymbol{2} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}; \; \boldsymbol{4}^{+} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}; \quad \boldsymbol{4}^{-} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix};$$

$$\boldsymbol{m}_{10} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \boldsymbol{m}_{01} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \; \boldsymbol{m}_{11} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}; \boldsymbol{m}_{1\bar{1}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

4.5 Character tables

4.5.1 Character table of *222*

222	*e*	*a*	*b*	*c*
A	1	1	1	1
$\mathbf{B}_1$	1	1	−1	−1
$\mathbf{B}_2$	1	−1	1	−1
$\mathbf{B}_3$	1	−1	−1	1

Character table of *32*

32	*1* (1)	*3* (2)	*2* (3)
$\mathbf{A}_1$	1	1	1
$\mathbf{A}_2$	1	1	−1
E	2	−1	0

4.5.2 Character table of *4*

4	*1*	*2*	4^{+}	4^{-}
A	1	1	1	1
B	1	1	−1	−1
$^1\mathbf{E}$	1	−1	$-i$	i
$^2\mathbf{E}$	1	−1	i	$-i$

Character table of *4mm*

4mm	*1* (1)	*2* (1)	*4* (2)	m_{01} (2)	m_{11} (2)
$\mathbf{A}_1$	1	1	1	1	1
$\mathbf{A}_2$	1	1	1	−1	−1
$\mathbf{B}_1$	1	1	−1	1	−1
$\mathbf{B}_2$	1	1	−1	−1	1
E	2	−2	0	0	0

4.5.3 Character table of *23*

The value of ϵ is $\exp 2\pi i/3$.

*emph*23	*e* (1)	*a* (3)	*q* (4)	q^2 (4)
A	1	1	1	1
$^1\mathbf{E}$	1	1	ϵ	ϵ^*
$^2\mathbf{E}$	1	1	ϵ^*	ϵ
T	3	−1	0	0

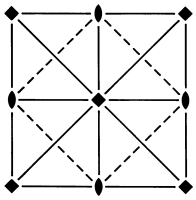
4.6 Space-group data

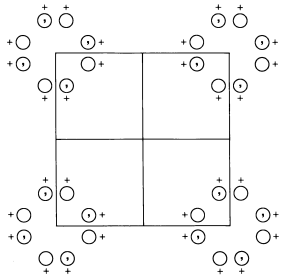
Figure 4.1: *IT*A space-group data for $P4mm$

International Tables for Crystallography (2016). Vol. A, Space group 99, p. 417.

Tetragonal $4mm$ C_{4v}^{1} $P4mm$

Patterson symmetry $P4/mmm$ $P4mm$ No. 99





Origin on $4mm$

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

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$
(5) m $x,0,z$ (6) m $0,y,z$ (7) m $x,\bar{x},z$ (8) m x,x,z

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	no conditions
							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl: $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

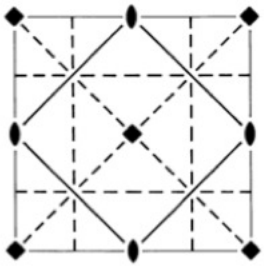
Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

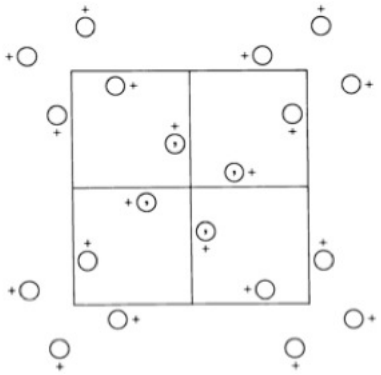
Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Figure 4.2: *IT*A space-group data for *P*4*bm* (selection)

P*4*bm C_{4v}^2 4*mm*

No. 100 *P*4*bm* Patterson syı





Origin on 4 1 *g*

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

Symmetry operations

(1) 1	(2) 2 0,0,*z*	(3) 4^+ 0,0,*z*	(4) 4^- 0,0,*z*
(5) *a* $x, \frac{1}{4}, z$	(6) *b* $\frac{1}{4}, y, z$	(7) *m* $x+\frac{1}{2}, \bar{x}, z$	(8) *g*$(\frac{1}{2}, \frac{1}{2}, 0)$ *x*,*x*,*z*

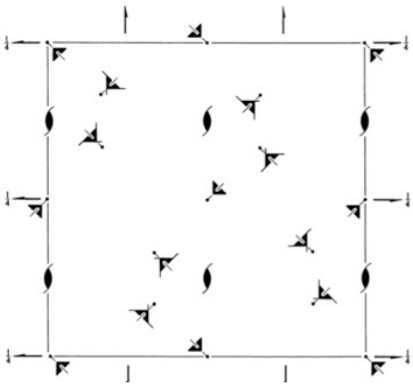
General position

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

Figure 4.3: *IT*A space-group data for $P2_13$ (selection)

$P2_13$ T^4 23 Cubic

No. 198 $P2_13$ Patterson symmetry $Pm\bar{3}$



Symmetry operations

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

(5) 3^+ x,x,x (6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$

(9) 3^- x,x,x (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

General position

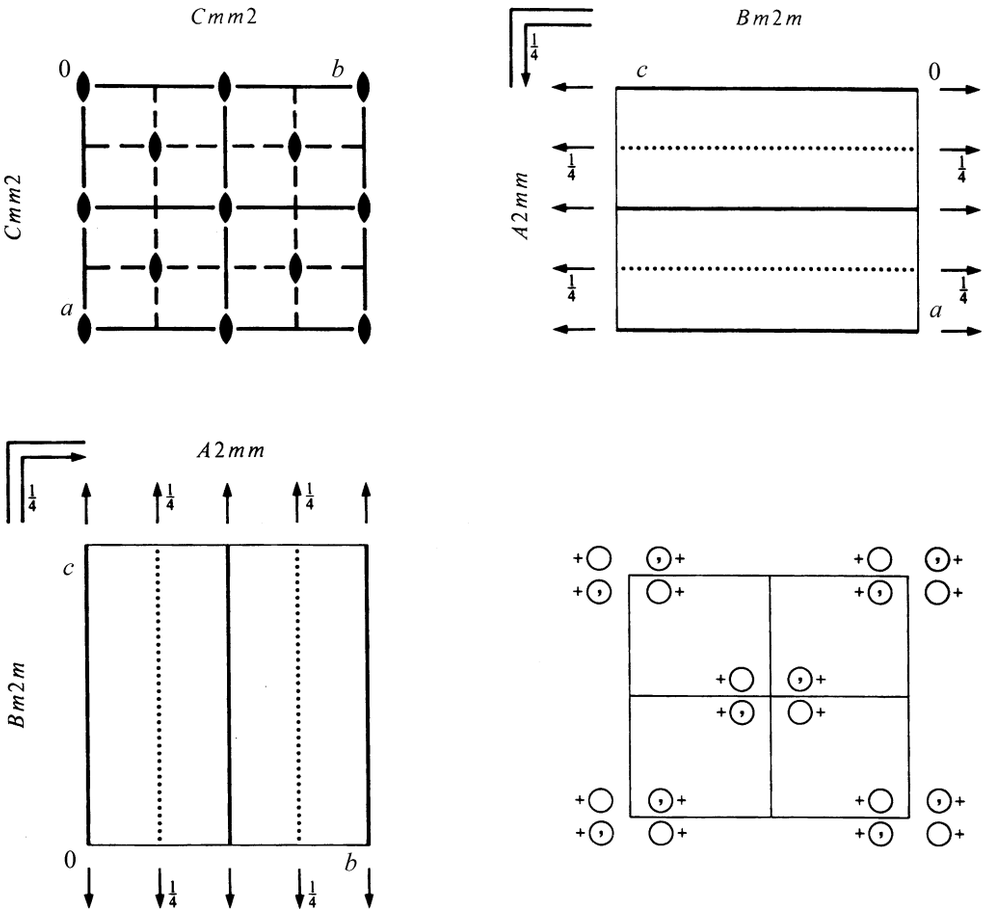
(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$

(5) z,x,y (6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$ (7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$ (8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$

(9) y,z,x (10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$ (11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$ (12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$

$Cmm2$ C_{2v}^{11} $mm2$ Orthorhombic

No. 35 $Cmm2$ Patterson symmetry $Cmmm$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	*f*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*e*	*m* . .	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	*d*	. *m* .	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	*c*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl: $h=2n$
2	*b*	*m m* 2	$0,\frac{1}{2},z$				no extra conditions
2	*a*	*m m* 2	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] *c* 2 *m m*
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

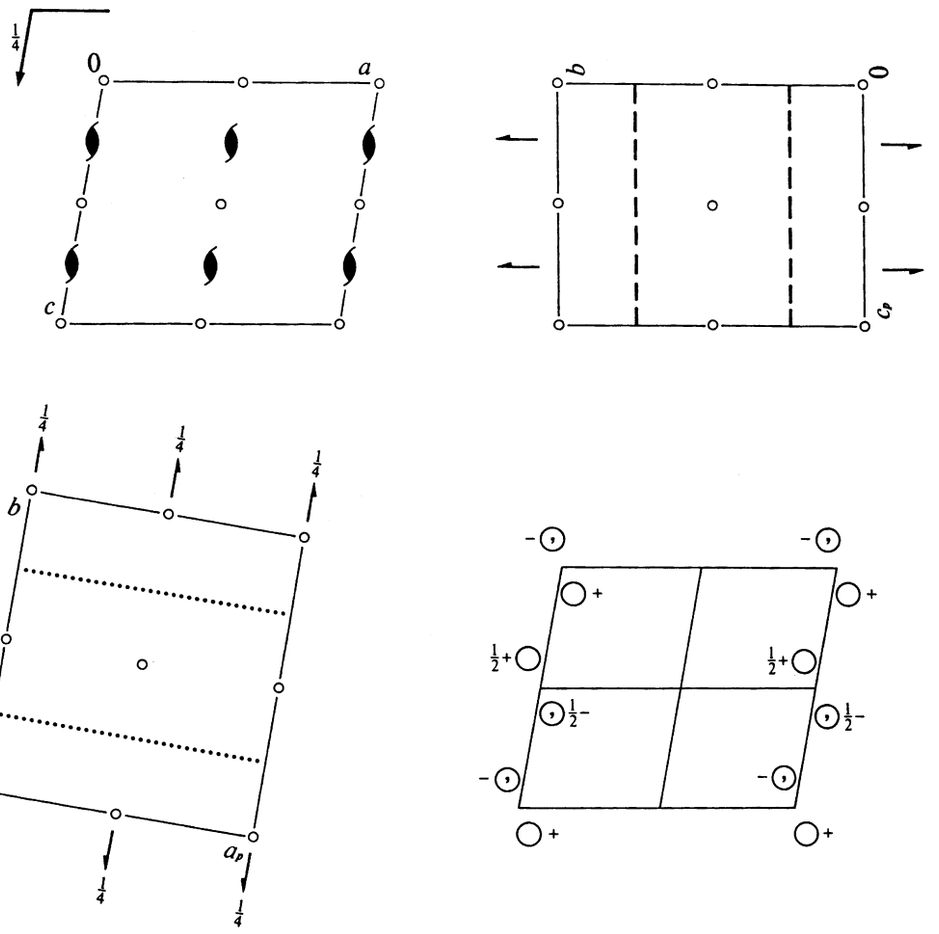
Along [100] *p* 1 *m* 1
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] *p* 1 1 *m*
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$P2_1/c$ 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 $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

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
							General:
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) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

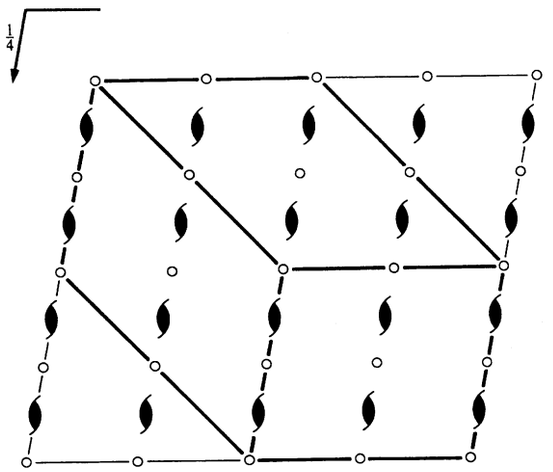
Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

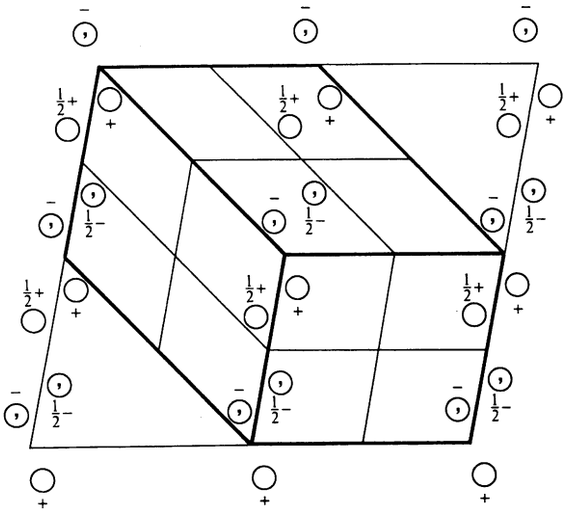
Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

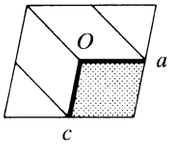
No. 14

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12_1/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$

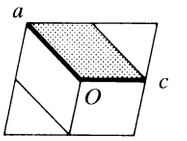
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

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

Positions

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

$P12_1/n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$

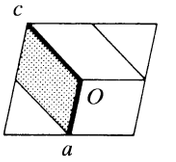
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $h+l=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $h+k+l=2n$
2	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

$P12_1/a1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$

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

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

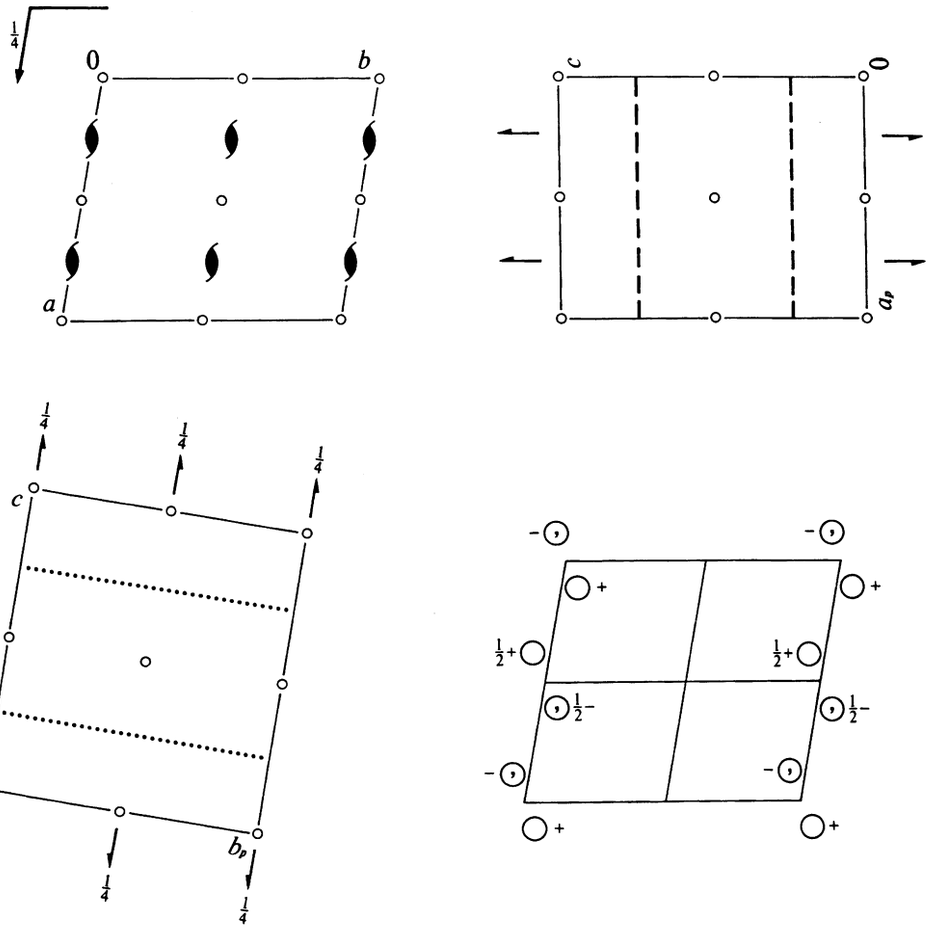
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	$h0l$: $h=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $h+k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

No. 14 $P112_1/a$

Patterson symmetry $P112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$

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

Symmetry operations

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

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
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0$: $h=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl: $h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+l=2n$

Symmetry of special projections

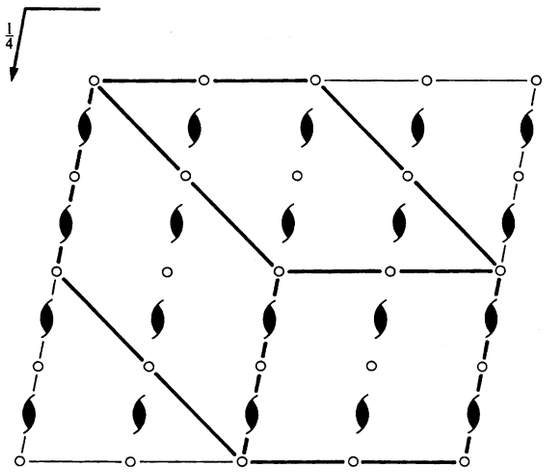
Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

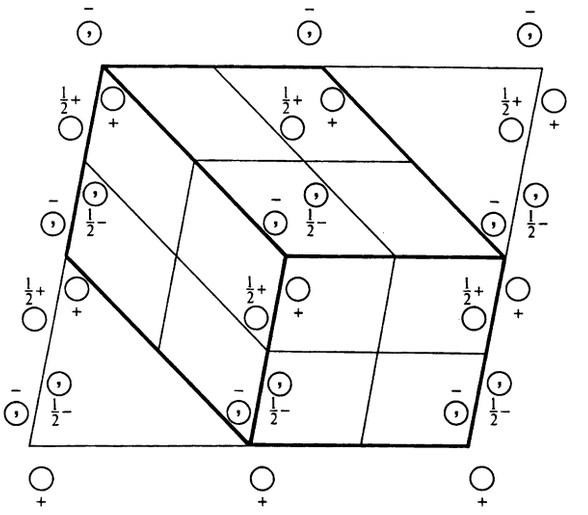
Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

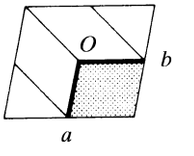
No. 14

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P112_1/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$

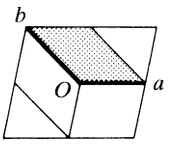
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

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
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0$: $h=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl: $h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+l=2n$

$P112_1/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$

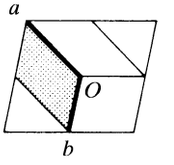
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

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
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

$P112_1/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$

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

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
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0$: $k=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$