Commission on Mathematical and Theoretical Crystallography

Summer Schools on Mathematical Crystallography

Representations of Crystallographic Groups

Nancy, France

June 28 - July 2, 2010

Contents

Contributing authors

Aroyo, Mois I.	Departamento de Física de la Materia Condensada, Universidad del País Vasco, E-48080 Bilbao, Spain
Capillas, César	Departamento de Física de la Materia Condensada, Universidad del País Vasco, E-48080 Bilbao, Spain
De la Flor, Gemma	Departamento de Física de la Materia Condensada, Universidad del País Vasco, E-48080 Bilbao, Spain
Kirov, Assen K.	Condensed Matter Physics Department, Sofia University, BG-1486 Sofia, Bulgaria
Orobengoa, Danel	Departamento de Física de la Materia Condensada, Universidad del País Vasco, E-48080 Bilbao, Spain
Perez-Mato, J. Manuel	Departamento de Física de la Materia Condensada, Universidad del País Vasco, E-48080 Bilbao, Spain
Wondraschek, Hans	Laboratorium für Applikationen der Synchrotronstrahlung, Karlsruher Institut für Technologie (KIT), D-76128 Karlsruhe, Germany

List of abbreviations

BC	Bradley, C. J. & Cracknell, A. P. (1972) The mathematical Theory of Symmetry in Solids. Oxford: Clarendon Press
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 (1983) Ed. Th. Hahn. 4th ed. (1996). Dordrecht: Kluwer Academic Publishers
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
$\mathcal{G}$, $\mathcal{H}$, *4*22	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

$\mathbf{D}$, $\mathbf{D}(\mathcal{G})$	rep, rep of group $\mathcal{G}$
$\mathbf{D}^{(i)}$	i-th irrep
$\chi(\mathbf{D})$	character of the rep $\mathbf{D}$
$\chi(\mathbf{D}^{(i)})$	character of the irrep $\mathbf{D}^{(i)}$
$O(\mathbf{D}^{(i)}(\mathcal{H}))$	Orbit of the irrep $\mathbf{D}^{(i)}$ of $\mathcal{H} \lhd \mathcal{G}$
$\mathcal{G}^i \equiv \mathcal{G}^i(\mathbf{D}^{(i)}(\mathcal{H})),\ \mathcal{H} \lhd \mathcal{G}$	little group
$\boldsymbol{D}(g)$	matrix of the rep $\mathbf{D}$, belonging to the group element g
$\boldsymbol{D}^{(i)}(g)$	matrix of the irrep $\mathbf{D}^{(i)}$, belonging to the group element g
$D^{(i)}(g)_{mn}$	m, n-th matrix element of the matrix $\boldsymbol{D}^{(i)}$ of irrep $\mathbf{D}^{(i)}$
$\dim(\mathbf{D}(\mathcal{G}))$	dimension of the rep $\mathbf{D}$
$\mathbf{D}^{(i)} \otimes \mathbf{D}^{(j)}$	direct product of irreps $\mathbf{D}^{(i)}$ and $\mathbf{D}^{(j)}$
$\mathbf{D}^{(i)} \oplus \mathbf{D}^{(j)}$	direct sum of irreps $\mathbf{D}^{(i)}$ and $\mathbf{D}^{(j)}$
m_j or $m(\mathbf{D} \,\vert\, \mathbf{D}^{(j)})$	multiplicity of the j-th irrep in the rep $\mathbf{D}$
$\mathbf{D}^{(i)}(\mathcal{G}) \downarrow \mathcal{H}$	irrep $\mathbf{D}^{(i)}(\mathcal{G})$ rep of group $\mathcal{H}$ subduced from the irrep $\mathbf{D}^{(i)}(\mathcal{G})$
$\mathbf{D}^{(i)}(\mathcal{H}) \uparrow \mathcal{G}$	rep of group $\mathcal{G}$, induced from the irrep $\mathbf{D}^{(i)}(\mathcal{H})$
$(\mathbf{D}^{(i)}(\mathcal{H}))_g$	irrep $\mathbf{D}^{(i)}(\mathcal{H}), \mathcal{H} \lhd \mathcal{G}$, 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 $\mathcal{T}$
$\mathbf{D}^{\mathbf{k},i}$	i-th (allowed) irrep of the little group $\mathcal{G}^{\mathbf{k}}$
$\mathbf{D}^{(\star\mathbf{k}),i}$	i-th irrep of the space group $\mathcal{G}$, belonging to $\star\mathbf{k}$
$\overline{\mathbf{D}}^{\mathbf{k},i}$	i-th irrep of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$

Part I

Irreducible representations of the crystallographic point and space groups

Mois I. Aroyo

Departamento Física de la Materia Condensada
Universidad del País Vasco, Bilbao, Spain
mois.aroyo@ehu.es

Hans Wondratschek

Laboratorium für Applikationen der Synchrotronstrahlung (LAS)
Universität, Karlsruhe, Germany
wondra@physik.uni-karlsruhe.de

The first part of the manuscript is devoted to a specific derivation of the irreducible representations (irreps) of the crystallographic point groups and space groups of 3-dimensional space. Following this procedure the readers should be able to derive these irreps themselves if necessary. Because of the restricted time and the practical goal of the school basic facts and theorems on representation theory could be only mentioned without proofs. For further studies the reader is referred to the literature given in the References.

After a brief introduction to crystallographic groups and their representations in the first two chapters, a general induction procedure for the derivation of the irreps of the crystallographic point groups is discussed in details in Chapter 3. The application of the same procedure for the derivation of the irreps of the crystallographic space groups is analyzed and demonstrated in the next Chapter 4. The accompanying exercises and the necessary data for the exercises like character tables of irreps, multiplication tables, *etc.* can be found in the last two chapters of Part I.

A Table of Contents and an Index will help the reader when studying the manuscript. A list of abbreviations and a list of symbols are also included.

The treatment of the irreps of one- and two-dimensional point and space groups is included in the treatment of the three-dimensional point and space groups because all groups of lower dimensions are represented under those of three dimensions. In four dimensions, however, there are point and space groups whose irreps can not be obtained by applying the methods used here. The icosahedral group which occurs in crystallographic point groups and thus in space groups of four dimensions is not a solvable group and, therefore, needs other procedures for the determination of its irreps.

This Part I of the manuscript is a slight modification of the lecture notes written by the authors for the course on Darstellungen der kristallographischen Punkt- und Raumgruppen, Hünfeld, 2000.

Chapter 1

Crystallographic point groups

In this chapter the group-theoretical aspect of the crystallographic point groups in three dimensions will be considered. Elementary notions of group theory are defined in the first section. They will be needed later. The crystallographic point groups are analyzed in the light of these definitions in the second section.

It is assumed that the reader is familiar with the crystallographic view of the point groups as groups of either the external shape and physical properties of macroscopic crystals or of the local symmetry in the crystal structure (site-symmetry groups). This includes a working knowledge of the Hermann-Mauguin (HM) and Schoenflies symbols of the point groups.

1.1 Special notions and results from group theory

In this section group-theoretical constructions and special types of groups are described which play a role for the irreps of the crystallographic point groups. The book of W. Ledermann is recommended.

- Conjugacy, subgroups, coset decomposition, and their consequences

  Let $\mathcal{G}$ be a finite group and $g_r \in \mathcal{G}$ be the elements of $\mathcal{G}$. The set of all elements $g_j = g_n^{-1} g_k g_n$, g_n running through the group $\mathcal{G}$, is called the *conjugacy class* of g_k. Elements of the same conjugacy class are called *conjugate*. The size of each conjugacy class, *i. e.* the number of its elements, divides the group order. Elements of the same conjugacy class have the same order. The unit element e forms always a conjugacy class for itself.

  Let $\mathcal{G}$ be a finite group and $\mathcal{U}= \{g_r \in \mathcal{G},\ r = 1,\ \ldots\ s\}$ a subset of elements of $\mathcal{G}$ which fulfill the group postulates for themselves. Then $\mathcal{U}$ is called a *subgroup* $\mathcal{U} < \mathcal{G}$.

  Let $\mathcal{G}$ be a finite group and $\mathcal{U} < \mathcal{G}$ a subgroup of $\mathcal{G}$. Then $\mathcal{G}$ can be *decomposed into left cosets* relative to $\mathcal{U}$: $\mathcal{G} = g_1\mathcal{U} \cup g_2\mathcal{U} \cup\ \ldots\ \cup g_i\mathcal{U}$,
  where $g_1 = e,\ g_2,\ \ldots,\ g_i$ are elements of $\mathcal{G}$ such that g_j does not occur in a coset of g_k with $k \neq j$. The elements g_j are called the *representatives* of their

cosets $g_j\mathcal{U}$. Any element $g_j u \in g_j\mathcal{U}, \quad u \in \mathcal{U}$ may represent the coset $g_j\mathcal{U}$. All cosets have the same number of elements as $\mathcal{U}$ has, and different cosets have no element in common. The number i of cosets is called the *index* $|\mathcal{G} : \mathcal{U}|$ of $\mathcal{U}$ in $\mathcal{G}$. Only the first coset, *i. e.* the subgroup itself, forms a subgroup of $\mathcal{G}$.

The decomposition can be made also from the right side (decomposition into right cosets): $\mathcal{G} = \mathcal{U} \cup \mathcal{U}\, g_2 \cup \ \ldots \ \cup \mathcal{U}\, g_i$.

Let $\mathcal{G}$ be a finite group and $\mathcal{U} < \mathcal{G}$ a subgroup of $\mathcal{G}$. Then $\mathcal{V} = g^{-1}\mathcal{U}\, g$ is a subgroup of $\mathcal{G}$ and is called *conjugate to* $\mathcal{U}$. The set of all subgroups of $\mathcal{G}$ which is obtained when g runs through $\mathcal{G}$ is called the *conjugacy class* of $\mathcal{U}$.

If $\mathcal{U}$ is mapped onto itself by all elements of $\mathcal{G}$, $g_n^{-1}\mathcal{U}\, g_n = \mathcal{U}$ for all $g_n \in \mathcal{G}$, then $\mathcal{U}$ is called a *normal subgroup* or *invariant subgroup* $\mathcal{U}$ of $\mathcal{G}$: $\mathcal{U} \lhd \mathcal{G}$. For a normal subgroup, right and left cosets are the same.

Lemma 1.1.1 If $\mathcal{N} \lhd \mathcal{G}$, then $\mathcal{N}$ contains with each element g also the full conjugacy class of g.

Normal subgroups play an important role if the homomorphic mapping of a group $\mathcal{G}$ onto a group $\mathcal{F}$ is considered.

Lemma 1.1.2 In a *homomorphic mapping* of a group $\mathcal{G}$ onto a group $\mathcal{F}$, a normal subgroup $\mathcal{N} \lhd \mathcal{G}$ is mapped onto the unit element $e \in \mathcal{F}$, and all elements of a coset of $\mathcal{G}$ relative to $\mathcal{N}$ are mapped onto one element $f_i \in \mathcal{F}$. Elements of different cosets are mapped on different elements $f_i \in \mathcal{F}$. The set of cosets relative to $\mathcal{N}$ forms a group which is isomorphic to $\mathcal{F}$ and is called the *factor group* or *quotient group* $\mathcal{G}/\mathcal{N}$ of $\mathcal{G}$ by $\mathcal{N}$.

- Cyclic groups

  In the following definition we make use of the abbreviation customary for products of identical group elements: $g\,g = g^2,\ g^2\,g = g\,g^2 = g^3,\ g^i\,g^k = g^k\,g^i = g^{i+k}$. If n is the smallest positive integer for which $g^n = e$ holds, e the unit element, then n is called the *order* of the element g, and one writes also g^{-i} for g^{n-i}.

  Definition (D 1.1.1) Let $\mathcal{G}$ be a group and $g \in \mathcal{G}$ an element of order n. The set $C_n = \{g = g_1,\ g^2 = g_2,\ g^3 = g_3, \ldots,\ g^{n-1} = g^{-1} = g_{n-1},\ g^n = e\}$ is called the *cyclic group of order n*, generated by g.

  Because of the validity of the associative law for the multiplication in the group, cyclic groups are always commutative: $g_i\,g_k = g_k\,g_i$. According to Table 1.2.1 there are five cyclic abstract groups to which ten crystal classes of point groups belong: $\mathcal{C}_1,\ \mathcal{C}_2,\ \mathcal{C}_3,\ \mathcal{C}_4,$ and $\mathcal{C}_6$.

- Abelian groups

  Definition (D 1.1.2) A group $\mathcal{G}$ is called an *Abelian group* if for all pairs of elements $g_i,\ g_k \in \mathcal{G}$ the relation $g_i\,g_k = g_k\,g_i$ holds.

Cyclic groups are always Abelian groups but not all Abelian groups are cyclic. There are four non-cyclic Abelian groups to which six of the 32 crystal classes belong, cf. Table 1.2.1 on p. 10: $\mathcal{D}_2$, $\mathcal{D}_{2h}$, $\mathcal{C}_{4h}$, and $\mathcal{C}_{6h}$.

To get an overview over the structure of the Abelian groups one uses the concept of the direct product.

Definition (D 1.1.3) A group $\mathcal{G}$ is called the *direct product* of its subgroups $\mathcal{U}$ and $\mathcal{V}$, $\mathcal{G} = \mathcal{U} \times \mathcal{V}$ if

1. $\mathcal{U} \lhd \mathcal{G}$ and $\mathcal{V} \lhd \mathcal{G}$ are normal subgroups of $\mathcal{G}$.
2. Every element $g \in \mathcal{G}$ can be written as a product of an element u of $\mathcal{U}$ and v of $\mathcal{V}$: $g = u\,v$.
3. The intersection of $\mathcal{U}$ and $\mathcal{V}$ is the unit element e of $\mathcal{G}$: $\mathcal{U} \cap \mathcal{V} = e$.

Equivalent to condition 1. is condition 1a:

1a. For each pair of elements $u \in \mathcal{U}$ and $v \in \mathcal{V}$ the commutative law holds, *i. e.* $u\,v = v\,u$ ($\mathcal{U}$ and $\mathcal{V}$ need not be Abelian groups).

Remark. If $g = u\,v$, then the elements $u \in \mathcal{U}$ and $v \in \mathcal{V}$ are uniquely determined.

Lemma 1.1.3 Basic Theorem for Abelian groups. Every finite Abelian group $\mathcal{G}$ is the direct product of *cyclic subgroups*. The order of $\mathcal{G}$ is the product of the orders of the cyclic subgroups.

In Table 1.2.1 the Abelian groups $\mathcal{D}_2$, $\mathcal{D}_{2h}$, $\mathcal{C}_{4h}$, and $\mathcal{C}_{6h}$ are written as the products of their cyclic factors. These factors are either the group $\mathcal{C}_2$ or the group $\mathcal{C}_3$, the cyclic groups of order 2 or 3.

Also non-Abelian groups can be direct products. According to Table 1.2.1 the groups $\mathcal{D}_6$, $\mathcal{D}_{4h}$, $\mathcal{D}_{6h}$, $\mathcal{T}_h$, and $\mathcal{O}_h$ are direct products, which are isomorphic to crystallographic groups. In all these cases one of the factors is $\mathcal{C}_2$.

- 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 1.1.4) 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 e only.

The relations between those abstract groups which are relevant for the three-dimensional point groups are displayed in the diagrams Fig. 1.1.1 and Fig. 1.1.2. One takes from these diagrams that the corresponding non-Abelian groups have the following composition series:

$\mathcal{D}_3 \rhd \mathcal{C}_3 \rhd \mathcal{I}$; $\mathcal{D}_4 \rhd \mathcal{C}_4 \rhd \mathcal{C}_2 \rhd \mathcal{I}$; $\mathcal{T} \rhd \mathcal{D}_2 \rhd \mathcal{C}_2 \rhd \mathcal{I}$; and $\mathcal{O} \rhd \mathcal{T} \rhd \mathcal{D}_2 \rhd \mathcal{C}_2 \rhd \mathcal{I}$.

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.

The generation of the abstract groups by composition series is displayed in Figs. 1.1.1 and 1.1.2. Each line connects a group - normal subgroup pair; each dashed arrow points to the direct product of the subgroup with the group $\mathcal{C}_2$. The number at the line is the index of the normal subgroup, *i. e.* the order of the factor group. The lines in $[\ \ldots\ ]$ are not necessary because they are contained in the framework: $\mathcal{C}_i \sim \mathcal{C}_2$, $\mathcal{C}_{2h} \sim \mathcal{D}_2$, $\mathcal{C}_{3i} \sim \mathcal{C}_6$, and $\mathcal{D}_{3d} \sim \mathcal{D}_6$. However, they make easier the transition to the corresponding diagrams 1.2.1 and 1.2.2.

Fig. 1.1.1 Generation of sub-cubic abstract groups, see Tab. 1.2.2

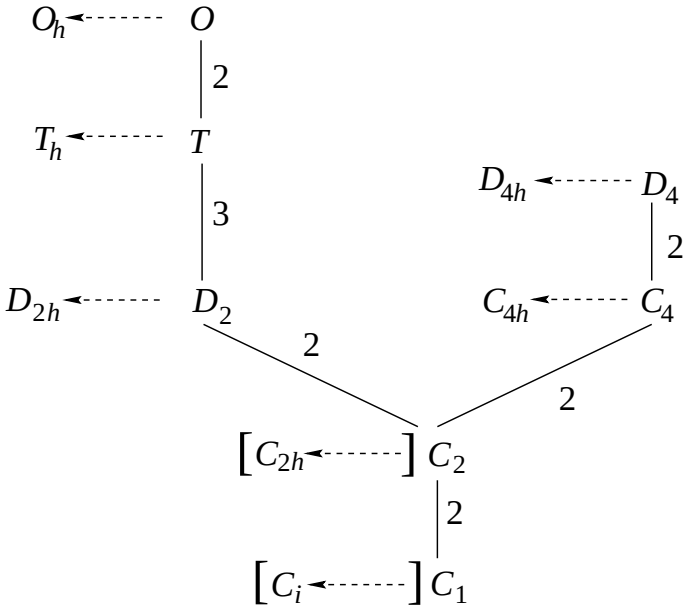
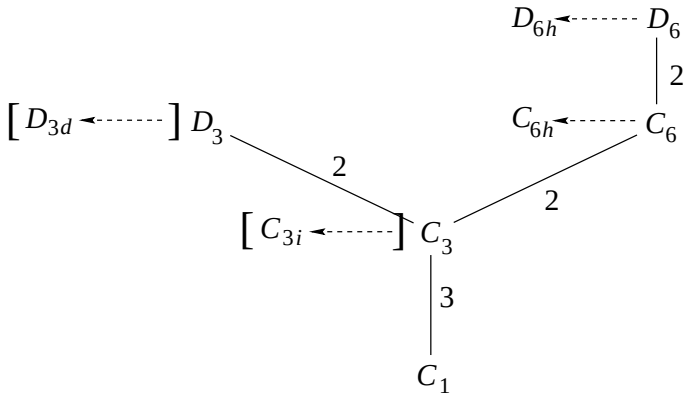


Fig. 1.1.2 Generation of sub-hexagonal abstract groups, see Tab. 1.2.3



1.2 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 1.2.1 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 1.2.1 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

---

The following diagrams correspond to the Figures 1.1.1 and 1.1.2. 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 $\overline{1}$. 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 1.2.2 and 1.2.3.

Fig. 1.2.1 Generation of sub-cubic point groups, see Tab. 1.2.2

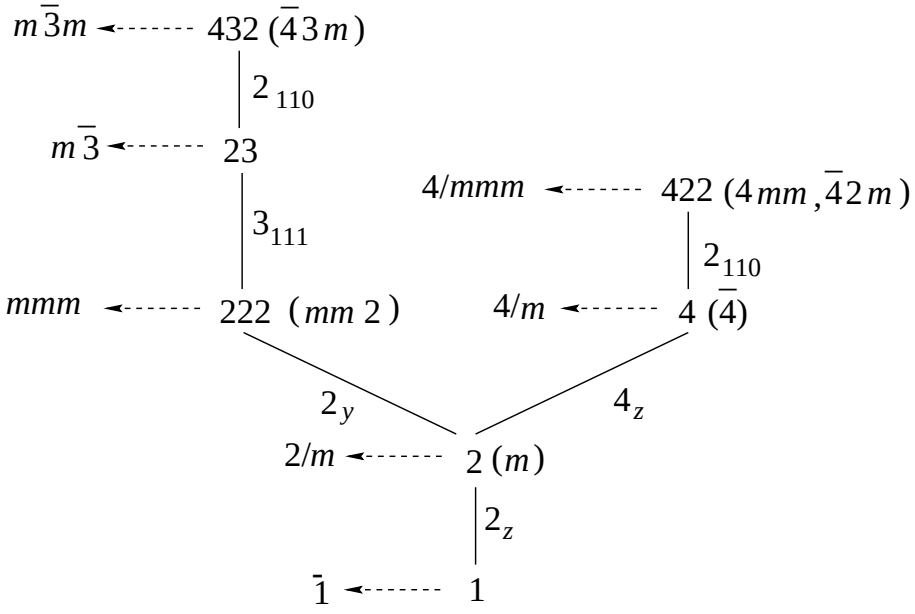


Fig. 1.2.2 Generation of sub-hexagonal point groups, see Tab. 1.2.3

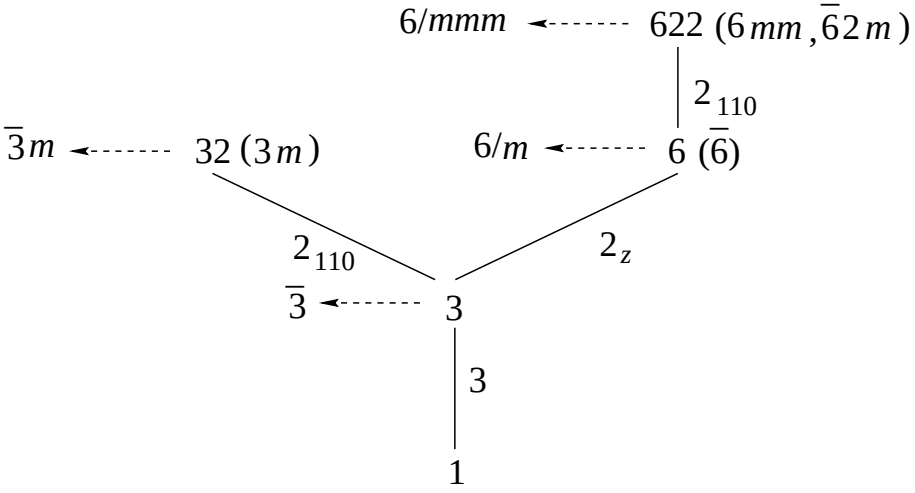


Table 1.2.2 The generation of the crystallographic point groups I

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. 1.2.1. 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.

Table 1.2.3 The generation of the crystallographic point groups II

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. 1.2.2. 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.

The composition series of Tables 1.2.2 and 1.2.3 seem to be natural but often they may be replaced by other composition series.

■ Examples.

$2/m \rhd 2 \rhd 1$ may be replaced by $2/m \rhd m \rhd 1$ or by $2/m \rhd \overline{1} \rhd 1$;
$4/m \rhd 4 \rhd 2 \rhd 1$ may be replaced by $4/m \rhd 2/m \rhd 2 \rhd 1$;
$4mm \rhd 4 \rhd 2 \rhd 1$ may be replaced by $4mm \rhd mm2 \rhd m \rhd 1$;
$622 \rhd 6 \rhd 3 \rhd 1$ may be replaced by $622 \rhd 32 \rhd 3 \rhd 1$;
$6/mmm \rhd 622 \rhd 6 \rhd 3 \rhd 1$ may be replaced by $6/mmm \rhd \overline{6}2m \rhd 3m \rhd 3 \rhd 1$; *etc.* ■

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. The procedure for the derivation of the irreps of these basic groups $\mathcal{D}_3,\ \mathcal{D}_4,\ \mathcal{T},$ and $\mathcal{O}$ is found in Chapter 3.

2.1 Representations

Definition (D 2.1.1) 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 $P\overline{4}3m$, 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 $g_m \to h_m,\ g_n \to h_n$, and $g_m\, g_n = g_{mn} \to h_{mn}$, 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 2.1.2) 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 2.1.3) 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 (proof ?).

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 2.1.4) 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 2.1.5) 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 1.2.1 on p. 10. 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 $D^{(ij)}(\mathsf{g})_{pq;rs} = D^{(i)}(\mathsf{h}_1)_{pr}\, D^{(j)}(\mathsf{h}_2)_{qs}$ where $\mathsf{g} = \mathsf{h}_1\, \mathsf{h}_2$. 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, see lemma 1.1.3 on p. 7, 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 $\mathcal{C}_n = \langle \mathsf{g} \rangle = \{\mathsf{e},\ \mathsf{g},\ \mathsf{g}^2,\ \ldots\ ,\ \mathsf{g}^{n-1}\}$ are given by the formula $\mathbf{D}^{(p)}(\mathsf{g}^m) = [\exp(2\,\pi\,i\,(p{-}1)/n)]^m = \exp(2\,\pi\,i\,m(p{-}1)/n),\ m,\ p = 1,\ 2,\ \ldots\ , n$.

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

2.2.2 The irreps of direct products of cyclic groups

According to lemma 1.1.3, 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 1.2.1 on p. 10. 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. 1.2.1 and 1.2.2.

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.

In the present manuscript the irreps of the non-Abelian groups are derived in Chapter 3 using a procedure which is based on the solvability of the crystallographic groups. 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.

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

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

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

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

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

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

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 $\boldsymbol{2}_z$ and $\boldsymbol{2}_y$ are represented by the unit matrix of $\mathbf{D}^{(3)}$. The generator $\boldsymbol{3}^+_{xxx}$ of $\mathcal{O}$ replaces the generator $\boldsymbol{3}^+_z$ of $\mathcal{D}_3$, and $\boldsymbol{m}_{xx}$ of $\mathcal{D}_3$ is replaced by $\boldsymbol{2}_{xx}$ in group 432 or by $\boldsymbol{m}_{xx}$ in group $\overline{4}3m$.

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

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

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

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

Chapter 3

Further development of representation theory

3.1 Definitions and general procedure

3.1.1 Subduced and induced representations

Let $\mathcal{H}$ be a proper subgroup of a group $\mathcal{G}$: $\mathcal{H} < \mathcal{G}$. Given an irrep $\mathbf{D}^{(r)}(\mathcal{G})$ of $\mathcal{G}$, one can construct a 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 3.1.1) Consider the set of matrices which form an irrep of $\mathcal{G}$. The set $\{\boldsymbol{D}^{(r)}(\boldsymbol{g}_i)\} = \mathbf{D}^{(r)}(\mathcal{G}) \downarrow \mathcal{H},\ \boldsymbol{g}_i \in \mathcal{H}$, is called the *representation of* $\mathcal{H}$ *subduced from* $\mathcal{G}$.

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

■ Examples.

1. It is trivial to state that any subduced rep of a one-dimensional irrep $\mathbf{D}^{(r)}(\mathcal{G})$ is one-dimensional again and thus irreducible.

2. Let $\mathbf{E}$ be the 2-dimensional irrep of the point group *4mm*:

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

$$\boldsymbol{m}_{yz} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \boldsymbol{m}_{xz} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \boldsymbol{m}_{x\overline{x}} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}; \boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

For the designation of the reflections, symbols are used which may apply for dimension 2 as well as for dimension 3: m_{yz} means the reflection in the plane $0yz$ or in the line $0y$, m_{xx} means the reflection in the plane xxz or in the line xx, *etc.*

The subduction to the rep of any subgroup of $4mm$ is reducible to one-dimensional constituents because any subgroup of $4mm$: 4, $m_{yz}m_{xz}2$, $m_{xx}m_{x\bar{x}}2$, *etc.* is an Abelian group. ■

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 $\mathcal{H}$:

$$\mathcal{G} = g_1\,\mathcal{H} \cup g_2\,\mathcal{H} \cup \ \ldots\ \cup g_r\,\mathcal{H} \qquad \text{with } g_1 = e. \tag{3.1}$$

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

$$\boldsymbol{D}^{Ind}(g)_{mt,ns} = \begin{cases} \boldsymbol{D}^{(j)}(g_m^{-1}\,g\,g_n)_{t,s} & \text{if } g_m^{-1}\,g\,g_n = h \in \mathcal{H} \\ 0 & \text{if } g_m^{-1}\,g\,g_n \notin \mathcal{H} \end{cases} \tag{3.2}$$

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

Definition (D 3.1.2) The representation of lemma 3.1.1 of $\mathcal{G}$ is called an *induced rep* of $\mathcal{G}$.

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

$$\boldsymbol{D}^{Ind}(g)_{mt,ns} = \boldsymbol{M}(g)_{m,n}\boldsymbol{D}^{(j)}(h)_{t,s}, \qquad \text{where } g_m^{-1}\,g\,g_n = h. \tag{3.3}$$

The matrix $\boldsymbol{M}(g)$ 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 $g_m^{-1}\,g\,g_n = h \in \mathcal{H}$. Correspondingly, the matrices $\boldsymbol{D}^{Ind}(g)$ have block structure with exactly one non-zero block in every column and every row, where the block is the matrix $\boldsymbol{D}^{(j)}(h)$, and h is fixed by the above condition.
Equation 3.2 is sometimes written in the form

$$\boldsymbol{D}^{Ind}(g) = \boldsymbol{M}(g) \otimes \boldsymbol{D}^{(j)}(h), \tag{3.4}$$

where the sign $\otimes$ is used for the construction in equation 3.4 although the matrix $\boldsymbol{D}^{(j)}(h)$ is different for different positions in $\boldsymbol{M}$.

In the following example reps of the point group $4mm$ are induced from the irreps of point group $1m1 = \{1,\ m_{xz}\}$.

■ Example. Reps of point group $4mm$ induced from the irreps of point group $1m1 = \{1,\ m_{xz}\}$.

1. Decomposition of $4mm$ relative to m_{xz}
   $4mm = \{1,\ m_{xz}\} \cup m_{yz}\{1,\ m_{xz}\} \cup 4_z\,\{1,\ m_{xz}\} \cup m_{x\bar{x}}\,\{1,\ m_{xz}\}$;
   coset representatives are $\{1,\ m_{yz},\ 4_z,$ and $m_{x\bar{x}}\}$.

2. Construction of the induction matrix $\boldsymbol{M}(g)$

   The induction matrix is constructed with the help of the group table of $4mm$.

Table 3.1.1 Group table of group $4mm$.

$4mm$	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\overline{x}}$
1	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\overline{x}}$
2_z	2_z	1	4_z^{-1}	4_z	m_{yz}	m_{xz}	$m_{x\overline{x}}$	m_{xx}
4_z	4_z	4_z^{-1}	2_z	1	m_{xx}	$m_{x\overline{x}}$	m_{yz}	m_{xz}
4_z^{-1}	4_z^{-1}	4_z	1	2_z	$m_{x\overline{x}}$	m_{xx}	m_{xz}	m_{yz}
m_{xz}	m_{xz}	m_{yz}	$m_{x\overline{x}}$	m_{xx}	1	2_z	4_z^{-1}	4_z
m_{yz}	m_{yz}	m_{xz}	m_{xx}	$m_{x\overline{x}}$	2_z	1	4_z	4_z^{-1}
m_{xx}	m_{xx}	$m_{x\overline{x}}$	m_{xz}	m_{yz}	4_z	4_z^{-1}	1	2_z
$m_{x\overline{x}}$	$m_{x\overline{x}}$	m_{xx}	m_{yz}	m_{xz}	4_z^{-1}	4_z	2_z	1

The columns of this table display the different steps in the determination of the non-zero elements of the matrix $\boldsymbol{M}$ and of the corresponding element $h \in \mathcal{H}$.
Col. 1: Element $g \in \mathcal{G}$ for which the rep matrix is to be determined;
Cols. 2 to 4: coset representative g_m, $m = 1 \ldots 4$ and steps towards the calculation of h;
Col. 5: listing of that (unique) coset representative which is necessary to obtain an element of $\mathcal{H}$;
Cols. 6 and 7 contain the element $h \in \mathcal{H}$ and the non-zero element of the row m of the $\boldsymbol{M}$ matrix which are needed for the next step.

g	g_m	g_m^{-1}	$g_m^{-1}\,g$	g_n	$h = g_m^{-1}\,g\,g_n$	$M_{mn} \neq 0$
1	1	1	1	1	1	M_{11}
	m_{yz}	m_{yz}	m_{yz}	m_{yz}	1	M_{22}
	4_z	4_z^{-1}	4_z^{-1}	4_z	1	M_{33}
	$m_{x\overline{x}}$	$m_{x\overline{x}}$	$m_{x\overline{x}}$	$m_{x\overline{x}}$	1	M_{44}
m_{xz}	1	1	m_{xz}	1	m_{xz}	M_{11}
	m_{yz}	m_{yz}	2_z	m_{yz}	m_{xz}	M_{22}
	4_z	4_z^{-1}	$m_{x\overline{x}}$	$m_{x\overline{x}}$	1	M_{34}
	$m_{x\overline{x}}$	$m_{x\overline{x}}$	4_z^{-1}	4_z	1	M_{43}
m_{yz}	1	1	m_{yz}	m_{yz}	1	M_{12}
	m_{yz}	m_{yz}	1	1	1	M_{21}
	4_z	4_z^{-1}	m_{xx}	4_z	m_{xz}	M_{33}
	$m_{x\overline{x}}$	$m_{x\overline{x}}$	4_z	$m_{x\overline{x}}$	m_{xz}	M_{44}
4_z	1	1	4_z	$m_{x\overline{x}}$	m_{xz}	M_{14}
	m_{yz}	m_{yz}	m_{xx}	4_z	m_{xz}	M_{23}
	4_z	4_z^{-1}	1	1	1	M_{31}
	$m_{x\overline{x}}$	$m_{x\overline{x}}$	m_{yz}	m_{yz}	1	M_{42}
$m_{x\overline{x}}$	1	1	$m_{x\overline{x}}$	$m_{x\overline{x}}$	1	M_{14}
	m_{yz}	m_{yz}	4_z^{-1}	4_z	1	M_{23}
	4_z	4_z^{-1}	m_{yz}	m_{yz}	1	M_{32}
	$m_{x\overline{x}}$	$m_{x\overline{x}}$	1	1	1	M_{41}

3. Construction of the induced reps $\mathbf{D}_i^{Ind}(4mm) = \mathbf{D}^{(i)}(m_{xz}) \uparrow 4mm,\ i = 1, 2$

   The matrices for the elements 1, m_{xz}, m_{yz}, 4, and $m_{x\overline{x}}$ are listed here. The elements 1 and m_{xz} form the subgroup $\mathcal{H}$, 4 can be taken as a generator which generates $\mathcal{G}$ from $\mathcal{H}$. The group $\mathcal{G}$ is also generated by m_{xz} and $m_{x\overline{x}}$, *etc.*

   One confirms for the listed matrices the relations $m_{xz}\,4 = m_{x\overline{x}}$ and $m_{x\overline{x}}\,m_{yz} = 4$, taken from the group table 3.1.1. The matrices for 2_z, 4_z^{-1}, and m_{xx} are calculated from those given by, *e. g.* $2_z = m_{xz}\,m_{yz}$, $4_z^{-1} = m_{yz}\,m_{x\overline{x}}$, and $m_{xx} = m_{yz}\,4_z$, following the group table 3.1.1.

$$\mathbf{D}_i^{Ind}(1) = \begin{pmatrix} \boldsymbol{D}^{(i)}(1) & 0 & 0 & 0 \\ 0 & \boldsymbol{D}^{(i)}(1) & 0 & 0 \\ 0 & 0 & \boldsymbol{D}^{(i)}(1) & 0 \\ 0 & 0 & 0 & \boldsymbol{D}^{(i)}(1) \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(m_{xz}) = \begin{pmatrix} \boldsymbol{D}^{(i)}(m_{xz}) & 0 & 0 & 0 \\ 0 & \boldsymbol{D}^{(i)}(m_{xz}) & 0 & 0 \\ 0 & 0 & 0 & \boldsymbol{D}^{(i)}(1) \\ 0 & 0 & \boldsymbol{D}^{(i)}(1) & 0 \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(m_{yz}) = \begin{pmatrix} 0 & \boldsymbol{D}^{(i)}(1) & 0 & 0 \\ \boldsymbol{D}^{(i)}(1) & 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{D}^{(i)}(m_{xz}) & 0 \\ 0 & 0 & 0 & \boldsymbol{D}^{(i)}(m_{xz}) \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(4_z) = \begin{pmatrix} 0 & 0 & 0 & \boldsymbol{D}^{(i)}(m_{xz}) \\ 0 & 0 & \boldsymbol{D}^{(i)}(m_{xz}) & 0 \\ \boldsymbol{D}^{(i)}(1) & 0 & 0 & 0 \\ 0 & \boldsymbol{D}^{(i)}(1) & 0 & 0 \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(m_{x\overline{x}}) = \begin{pmatrix} 0 & 0 & 0 & \boldsymbol{D}^{(i)}(1) \\ 0 & 0 & \boldsymbol{D}^{(i)}(1) & 0 \\ 0 & \boldsymbol{D}^{(i)}(1) & 0 & 0 \\ \boldsymbol{D}^{(i)}(1) & 0 & 0 & 0 \end{pmatrix}.$$

■

3.1.2 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 3.1.3) 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 $\mathbf{H}$ 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 3.1.4) 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:
$(\mathbf{D}^{(s)}(h))_{g'_i} = \mathbf{D}^{s}(g_i'^{-1}\,h\,g'_i) = \mathbf{D}^{(s)}(h'^{-1}\,g_i^{-1}\,h\,g_i\,h') = \mathbf{D}^{(s)}(h'^{-1})\,\mathbf{D}^{(s)}(g_i^{-1}\,h\,g_i)\,\mathbf{D}^{(s)}(h') = \mathbf{D}^{(s)}(h')^{-1}(\mathbf{D}^{(s)}(h))_{g_i}\mathbf{D}^{(s)}(h')$, 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 3.1.3.

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 $\mathcal{H}$.

■ Example 1. Distribution of the irreps of 4 into orbits of conjugate irreps relative to $4mm$

- Coset decomposition of $4mm$ relative to 4
  $4mm = 4 \cup m_{xz}\,4$

- Conjugation of the elements of 4 under m_{xz}
  $m_{xz}^{-1}\, 4_z\, m_{xz} = 4_z^{-1}$; $\quad m_{xz}^{-1}\, 2_z\, m_{xz} = 2_z$

- irreps of 4 and their conjugacy by m_{xz}
  From the conjugation of the elements of 4 it follows that the conjugate of an irrep $\{\boldsymbol{D}^{(i)}(1),\ \boldsymbol{D}^{(i)}(4_z),\ \boldsymbol{D}^{(i)}(2_z),\ \boldsymbol{D}^{(i)}(4_z^{-1})\}$ is obtained by the following mapping:
  $1 \to \boldsymbol{D}^{(i)}(1)$, $\quad 2_z \to \boldsymbol{D}^{(i)}(2_z)$, $\quad 4_z \to \boldsymbol{D}^{(i)}(4_z^{-1})$, $\quad 4_z^{-1} \to \boldsymbol{D}^{(i)}(4_z)$.

Irreps of 4

4	1	4_z	2_z	4_z^{-1}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	i	-1	$-i$
$\mathbf{D}^{(4)}$	1	$-i$	-1	i

Irreps of 4 conjugated by $m_{xz} \in 4mm$

4	1	4_z	2_z	4_z^{-1}
$(\mathbf{D}^{(1)})_{m_{xz}}$	1	1	1	1
$(\mathbf{D}^{(2)})_{m_{xz}}$	1	-1	1	-1
$(\mathbf{D}^{(3)})_{m_{xz}}$	1	$-i$	-1	i
$(\mathbf{D}^{(4)})_{m_{xz}}$	1	i	-1	$-i$

.

The irreps $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are self-conjugate because $(\mathbf{D}^{(1)})_{m_{xz}} = \mathbf{D}^{(1)}$ and $(\mathbf{D}^{(2)})_{m_{xz}} = \mathbf{D}^{(2)}$, while $\mathbf{D}^{(3)}$ and $\mathbf{D}^{(4)}$ form a pair of conjugate irreps. The orbits are $\{\mathbf{D}^{(1)}\}$, $\{\mathbf{D}^{(2)}\}$, $\{\mathbf{D}^{(3)},\ \mathbf{D}^{(4)}\}$. ■

■ Example 2. Distribution of the irreps of $mm2$ into orbits of conjugate irreps relative to $4mm$.

- coset decomposition
  $4mm = mm2 \cup 4_z\, mm2$

- conjugation of the elements of $mm2$ under 4_z
  $4_z^{-1}\, m_{xz}\, 4_z = m_{yz}$; $\ 4_z^{-1}\, m_{yz}\, 4_z = m_{xz}$; $\ 4_z^{-1}\, 2_z\, 4_z = 2_z$.

- irreps of $mm2$ and their conjugates under 4_z

$mm2$	1	m_{xz}	m_{yz}	2_z
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	1	-1	-1
$\mathbf{D}^{(3)}$	1	-1	1	-1
$\mathbf{D}^{(4)}$	1	-1	-1	1

$mm2$	1	m_{xz}	m_{yz}	2_z
$(\mathbf{D}^{(1)})_{4_z}$	1	1	1	1
$(\mathbf{D}^{(2)})_{4_z}$	1	-1	1	-1
$(\mathbf{D}^{(3)})_{4_z}$	1	1	-1	-1
$(\mathbf{D}^{(4)})_{4_z}$	1	-1	-1	1

.

- orbits of irreps of $mm2$ under the group $4mm$; $\{\mathbf{D}^{(1)}\}$, $\{\mathbf{D}^{(2)},\ \mathbf{D}^{(3)}\}$, $\{\mathbf{D}^{(4)}\}$ ■

■ Example 3. Orbits of irreps of a non-centro-symmetric group $\mathcal{G}$ relative to the corresponding group $\mathcal{G} \times \overline{1}$, where $\overline{1}$ is the inversion group $\overline{1} = \{1,\ \overline{1}\}$

- coset decomposition of $\mathcal{G} \times \overline{1}$ relative to $\mathcal{G}$
  $\mathcal{G} \times \overline{1} = \mathcal{G} \cup \overline{1}\,\mathcal{G}$.

As the inversion commutes with all $g \in \mathcal{G}$, all irreps of $\mathcal{G}$ are self-conjugate in $\mathcal{G} \times \overline{1}$.■

3.1.3 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 3.1.5) 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 3.1.6) 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 3.1.2 **Induction Theorem**

1. 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 $O(\mathbf{D}^{(j)}(\mathcal{H}))$.

2. All irreps of $\mathcal{G}$ are obtained exactly once if the procedure described in 1 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. For each of them a series of subgroups $\mathcal{H}_i$ exists such that

$$\mathcal{G} \rhd \mathcal{H}_1 \rhd \ldots \rhd \mathcal{H}_{k-1} \rhd \mathcal{H}_k \rhd \ldots \rhd \mathcal{H}_n = \mathcal{I} \tag{3.5}$$

with $\mid \mathcal{H}_{k-1}/\mathcal{H}_k \mid = 2$ or 3, *i. e.* with cyclic factor groups of order 2 or 3.

3.2 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.* $\mathcal{G}^s(\mathbf{D}^{(s)}(\mathcal{H})) = \mathcal{G}$.

3.2.1 The induction formulae for 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 3.1.1.

For example, for index 2 the auxiliary table necessary for the construction of the induced irrep has the form, *cf.* the table in Section 3.1.1

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 $\mathbf{D}^{Ind}(\mathcal{G})$:

$$\mathbf{D}^{Ind}(h) = \begin{pmatrix} \boldsymbol{D}^{(s)}(h) & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_q \end{pmatrix};\ \mathbf{D}^{Ind}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{D}^{(s)}(q^2) \\ \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}. \tag{3.6}$$

Similarly, the general procedure reduces for index 3:

$$\mathbf{D}^{Ind}(h) = \begin{pmatrix} \boldsymbol{D}^{(s)}(h) & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_q & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_{q^2} \end{pmatrix};\mathbf{D}^{Ind}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{D}^{(s)}(q^3) \\ \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}. \tag{3.7}$$

From the induction theorem on p. 28 follows that each orbit of conjugate irreps of $\mathcal{H}$ yields exactly one irrep of $\mathcal{G}$.

Remark. In accordance with lemma 2.1.6, by subduction from $\mathcal{G}$ to $\mathcal{H}$ all two or three conjugate irreps of $\mathcal{H}$ 'appear'. The (square of) the dimension compensates the 'loss' of irreps in the induction and takes account of the increase of group order from $\mathcal{H}$ to $\mathcal{G}$.

3.2.2 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

$$\boldsymbol{D}^{(s),1}(h) = \boldsymbol{D}^{(s),2}(h) = \boldsymbol{D}^{(s)}(h),\ h \in \mathcal{H} \qquad \boldsymbol{D}^{(s),1}(q) = -\boldsymbol{D}^{(s),2}(q) = \boldsymbol{U} \tag{3.8}$$

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

$$\boldsymbol{D}^{(s),m}(h) = \boldsymbol{D}^{(s)}(h),\ m = 1,\ 2,\ 3 \qquad \boldsymbol{D}^{(s),1}(q) = \epsilon\boldsymbol{D}^{(s),2}(q) = \epsilon^2\boldsymbol{D}^{(s),3}(q) = \boldsymbol{U} \tag{3.9}$$

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

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

3.3 Examples

The following examples give the opportunity to apply the formulae 3.6, 3.7, 3.8, and 3.9.

3.3.1 Example 1

Determination of the irreps of the group $\mathcal{C}_4$.

The group $\mathcal{C}_4$ is an Abelian group. Therefore, all subgroups are normal subgroups, all irreps of $\mathcal{C}_4$ and of its subgroups are of dimension 1, *i. e.* they are (complex) numbers, and all orbits of irreps have the length 1. In all cases, formula 3.8 applies.

The composition series of the group $\mathcal{C}_4$ is $\mathcal{C}_4 \rhd \mathcal{C}_2 \rhd \mathcal{C}_1$.

Decomposition of the group $\mathcal{C}_2$ relative to its subgroup $\mathcal{C}_1$: $\mathcal{C}_2 = \mathcal{C}_1 \cup b\,\mathcal{C}_1$. The coset representative q of formula 3.8 is the element b.
Determination of the matrix $\boldsymbol{U}$:

1. $\boldsymbol{U}^{-1}\boldsymbol{A}(e)\,\boldsymbol{U} = \boldsymbol{1}$: self-conjugacy; $\boldsymbol{U} = e^{i\phi}$ (Schur's lemma).
2. $\boldsymbol{U}^2 = \boldsymbol{A}(e) = 1$; $\boldsymbol{U} = \pm 1$.

The irreps of the group $\mathcal{C}_2$ are

$\mathcal{C}_2$	e	b
A	1	1
B	1	−1

.

The decomposition of the $\mathcal{C}_4$ relative to its subgroup $\mathcal{C}_2$ is $\mathcal{C}_4 = \mathcal{C}_2 \cup a\,\mathcal{C}_2$.

Group table of the group $\mathcal{C}_4$:

$\mathcal{C}_4$	e	a	a^2	a^3
e	e	a	a^2	a^3
a	a	a^2	a^3	e
a^2	a^2	a^3	e	a
a^3	a^3	e	a	a^2

; the form

$\mathcal{C}_4$	e	a^2	a	a^3
e	e	a^2	a	a^3
a^2	a^2	e	a^3	a
a	a	a^3	a^2	e
a^3	a^3	a	e	a^2

is more transparent for our purpose because it accentuates the subgroup $\mathcal{C}_2$. The elements of $\mathcal{C}_2$ are e and $a^2 = b$; the new generator is $q = a$. Because $\mathcal{C}_4$ is Abelian, $q^{-1}a^2q = a^2$ holds. The orbits of the irreps of $\mathcal{C}_2$ relative to $\mathcal{C}_4$ are self-conjugate, *i. e.* $O(\mathbf{A}) = \mathbf{A}$; $O(\mathbf{B}) = \mathbf{B}$.

1. The irreps of the group $\mathcal{C}_4$, induced from the irrep **A**. One determines the matrix $\boldsymbol{U}$ for $O(\mathbf{A})$:

   (a) $\boldsymbol{U}^{-1}\,\boldsymbol{A}(h)\,\boldsymbol{U} = \boldsymbol{A}(h)$, $h \in \mathcal{C}_2$: self-conjugacy; $\boldsymbol{U} = e^{i\phi}$ (Schur's lemma).
   (b) $\boldsymbol{U}^2 = \boldsymbol{A}(q^2) = \boldsymbol{A}(a^2) = +1$; $\boldsymbol{U} = \pm 1$.

   From the irrep **A** of $\mathcal{C}_2$ the irreps **A** and **B** of $\mathcal{C}_4$ have been induced, see Table 3.3.1.

2. The irreps of $\mathcal{C}_4$, induced from the irrep **B** of $\mathcal{C}_2$. One calculates the matrix $\boldsymbol{U}$ by

   (a) $\boldsymbol{U}^{-1}\,\boldsymbol{B}(h)\,\boldsymbol{U} = \boldsymbol{B}(h)$, $h \in \mathcal{C}_2$: self-conjugacy; $\boldsymbol{U} = e^{i\phi}$ (Schur's lemma).
   (b) $\boldsymbol{U}^2 = \boldsymbol{B}(q^2) = \boldsymbol{B}(a^2) = -1$; $\boldsymbol{U} = \pm i$.

From the irrep **B** of $\mathcal{C}_2$ the irreps ${}^1\mathbf{E}$ and ${}^2\mathbf{E}$ of $\mathcal{C}_4$ are induced. All four irreps are listed in the following table.

Table 3.3.1 Irreps of $\mathcal{C}_4$

$\mathcal{C}_4$	e	a^2	a	a^3
A	1	1	1	1
B	1	1	-1	-1
${}^1\mathbf{E}$	1	-1	$-i$	i
${}^2\mathbf{E}$	1	-1	i	$-i$

3.3.2 Example 2

Determination of the irreps of the group $\mathcal{T}$ (Tetrahedral group of order 12), induced from the irreps of the group $\mathcal{D}_2$. The crystallographic realizations of these groups are the point groups (denoted by their HM symbols) 23 and 222.

The composition series of $\mathcal{T}$ is $\mathcal{T} \rhd \mathcal{D}_2 \rhd \mathcal{C}_2 \rhd \mathcal{C}_1$

The irreps of the group $\mathcal{T}$ will be derived from the irreps of its normal subgroup $\mathcal{D}_2$.

The irreps of $\mathcal{D}_2$ are

$\mathcal{D}_2$	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

1. Determination of the orbits of the irreps of $\mathcal{D}_2$ relative to the tetrahedral group $\mathcal{T}$:

   The coset decomposition of $\mathcal{T}$ relative to $\mathcal{D}_2$ is $\mathcal{T} = \mathcal{D}_2 \cup q\,\mathcal{D}_2 \cup q^2\,\mathcal{D}_2$, where the elements q and q^2 are found in the group table 3.3.2 of $\mathcal{T}$. The group $\mathcal{D}_2$ is displayed in the upper left square of the table; the generator q has the same name in the group table.

   One takes from the group table 3.3.2 of $\mathcal{T}$ the results of the conjugation of the elements of $\mathcal{D}_2$

conjugation relations in the group $\mathcal{T}$
$q^{-1}\,eq = e$; $q^{-2}\,eq^2 = e$;
$q^{-1}\,aq = b$; $q^{-2}\,aq^2 = c$;
$q^{-1}\,bq = c$; $q^{-2}\,bq^2 = a$;
$q^{-1}\,cq = a$; $q^{-2}\,cq^2 = b$.

$\mathcal{T}$	e	a	b	c	q	r	s	t	q^2	r^2	s^2	t^2
e	e	a	b	c	q	r	s	t	q^2	r^2	s^2	t^2
a	a	e	c	b	t	s	r	q	s^2	t^2	q^2	r^2
b	b	c	e	a	r	q	t	s	t^2	s^2	r^2	q^2
c	c	b	a	e	s	t	q	r	r^2	q^2	t^2	s^2
q	q	s	t	r	q^2	s^2	t^2	r^2	e	b	c	a
r	r	t	s	q	t^2	r^2	q^2	s^2	b	e	a	c
s	s	q	r	t	r^2	t^2	s^2	q^2	c	a	e	b
t	t	r	q	s	s^2	q^2	r^2	t^2	a	c	b	e
q^2	q^2	t^2	r^2	s^2	e	c	a	b	q	t	r	s
r^2	r^2	s^2	q^2	t^2	c	e	b	a	s	r	t	q
s^2	s^2	r^2	t^2	q^2	a	b	e	c	t	q	s	r
t^2	t^2	q^2	s^2	r^2	b	a	c	e	r	s	q	t

Table 3.3.2 Group table of group $\mathcal{T}$. The elements of the group table have the orders
order 1: e
order 2: a, b, c
order 3: q, r, s, t, q^2, r^2, s^2, t^2.

The orbits of irreps of $\mathcal{D}_2$ are $O(\mathbf{A}) = (\mathbf{A})$; $O(\mathbf{B}_1) = \{\mathbf{B}_1,\ \mathbf{B}_2,\ \mathbf{B}_3\}$.

2. Irreps of the group $\mathcal{T}$

   The irrep $\mathbf{A}$ is self-conjugate. The lemma of Schur applies: $\boldsymbol{U} = \exp(i\phi)$. For the determination of the matrix $\boldsymbol{U}$ only the equation $\boldsymbol{U}^3 = \mathbf{A}(q^3) = \mathbf{1} = 1$ remains. The result is $\boldsymbol{U}_m = \exp 2\pi i m/3$, $m = 1$, 2, and 3. From the irrep $\mathbf{A}$ of group 222 the three irreps $\mathbf{A}$, ${}^1\mathbf{E}$, and ${}^2\mathbf{E}$ are induced.

   The orbit $O(\mathbf{B}_1)$ consists of three irreps, thus formula 3.7 applies. One obtains the following matrices for the fourth irrep of $\mathcal{T}$:

$$\boldsymbol{T}(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix};\ \boldsymbol{T}(a) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix};\ \boldsymbol{T}(b) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

$$\boldsymbol{T}(c) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix};\ \boldsymbol{T}(q) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

   The matrices for the other elements of $\mathcal{T}$ are obtained by multiplication of these matrices according to the group table, for example
   $\boldsymbol{T}(q^2) = \boldsymbol{T}(q)\,\boldsymbol{T}(q)$;
   $\boldsymbol{T}(r) = \boldsymbol{T}(b)\,\boldsymbol{T}(q)$; $\boldsymbol{T}(s^2) = \boldsymbol{T}(a)\,\boldsymbol{T}(q^2)$; *etc.*

The characters of the irreps of $\mathcal{T}$ are given in Section 6.4.3, page 57.

Chapter 4

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 $\mathcal{H} \lhd \mathcal{G}$ which has been discussed and demonstrated for 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 4.1. The determination of the little groups of the selected irreps (step 3) and the induction procedure (step 5) follow the general scheme already explained and applied in the derivation of the point-group irreps. 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.

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

For representation theory we follow the terminology of BC and CDML.

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

$$(\boldsymbol{I},\ \boldsymbol{t}_i)^{N_i} = (\boldsymbol{I},\ \boldsymbol{N}_i) = (\boldsymbol{I},\ \boldsymbol{o}) \tag{4.1}$$

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 ($\boldsymbol{I}$, $\boldsymbol{t}$)

$$(\boldsymbol{I},\ \boldsymbol{N}\,\boldsymbol{t}) = (\boldsymbol{I},\ \boldsymbol{o}) \qquad \text{holds,} \tag{4.2}$$

where $\boldsymbol{N}\,\boldsymbol{t}$ is the column $(N_1 n_1, N_2 n_2, N_3 n_3)$. 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, *cf.* Lomont (1959), Jansen & Boon (1967). 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 (4.1) and (4.2) the irreps $\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\ \boldsymbol{t})]$ of $\mathcal{T}$ have the form

$$\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\ \boldsymbol{t})] = e^{-2\pi i (q_1 \frac{n_1}{N_1} + q_2 \frac{n_2}{N_2} + q_3 \frac{n_3}{N_3})}, \tag{4.3}$$

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

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \tag{4.4}$$

where $\mathbf{a} \cdot \mathbf{a}^*$ means the scalar product between the vectors, and δ_{ij} is the unit matrix (see, *e.g.*, IT B, 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:

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}. \tag{4.5}$$

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],

$$\mathbf{K} = K_1\mathbf{a}_1^* + K_2\mathbf{a}_2^* + K_3\mathbf{a}_3^*, \tag{4.6}$$

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, Chapter 5, the basis of direct space is denoted by a row $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}$, where $(\ )^{\mathrm{T}}$ means transposed relative to columns. For the reciprocal space, the basis is described by a column $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*)$.

To each lattice generated from a basis $(\mathbf{a}_i)^{\mathrm{T}}$ a reciprocal lattice is generated from the basis $(\mathbf{a}_j^*)$. Both lattices, $\mathbf{L}$ and $\mathbf{L}^*$, can be compared most easily by referring the direct lattice $\mathbf{L}$ to its *conventional basis* $(\mathbf{a}_i)^{\mathrm{T}}$ as defined in Sections 2.1 and 9.1 of IT A. In this case the lattice $\mathbf{L}$ may be primitive or centred. If $(\mathbf{a}_i)^{\mathrm{T}}$ forms a primitive basis of $\mathbf{L}$, *i.e.* if $\mathbf{L}$ is primitive, then the basis $(\mathbf{a}_j^*)$ forms a primitive basis of $\mathbf{L}^*$. If $\mathbf{L}$ is centred, *i.e.* $(\mathbf{a}_i)^{\mathrm{T}}$ is not a primitive basis of $\mathbf{L}$, then there exists a centring matrix $\boldsymbol{P}$, $0 < \det(\boldsymbol{P}) < 1$, by which three linearly independent vectors of $\mathbf{L}$ with rational coefficients are generated from those with integer coefficients, *cf.* IT A, Table 5.1.

Moreover, $\boldsymbol{P}$ can be chosen such that the set of vectors

$$(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^{\mathrm{T}} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}\,\boldsymbol{P} \tag{4.7}$$

forms a primitive basis of $\mathbf{L}$. Then the basis vectors $(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*)$ of the lattice reciprocal to the lattice generated by $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^{\mathrm{T}}$ are determined by

$$(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*) = \boldsymbol{P}^{-1}(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*) \tag{4.8}$$

and form a primitive basis of $\mathbf{L}^*$.

Because of $\det(\boldsymbol{P}^{-1}) > 1$ not all vectors $\mathbf{K}$ of the form (4.6) belong to $\mathbf{L}^*$. If $k_{p1}\mathbf{p}_1^* + k_{p2}\mathbf{p}_2^* + k_{p3}\mathbf{p}_3^*$ are the vectors of $\mathbf{L}^*$ and $K_1,\ K_2,\ K_3$ are the (integer) coefficients of these vectors $\mathbf{K}$ referred to $(\mathbf{a}_j^*)$, then $\mathbf{K} = (K_j)^{\mathrm{T}}\ (\mathbf{a}_j^*) = (K_j)^{\mathrm{T}}\,\boldsymbol{P}(\mathbf{p}_i^*) = (k_{pi})^{\mathrm{T}}\ (\mathbf{p}_i^*)$ is a vector of $\mathbf{L}^*$ if and only if the coefficients

$$(k_{p1}, k_{p2}, k_{p3})^{\mathrm{T}} = (K_1, K_2, K_3)^{\mathrm{T}}\boldsymbol{P} \tag{4.9}$$

are integers. In other words, $(K_1,\ K_2,\ K_3)^{\mathrm{T}}$ has to fulfill the equation

$$(K_1, K_2, K_3)^{\mathrm{T}} = (k_{p1}, k_{p2}, k_{p3})^{\mathrm{T}}\boldsymbol{P}^{-1}. \tag{4.10}$$

[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 (4.4) and (4.5) 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 $(\mathbf{a}_i)^{\mathrm{T}}$, then $\boldsymbol{W}^{-1}$ is the matrix of the same symmetry operation of the reciprocal lattice but referred to the dual basis $(\mathbf{a}_i^*)$. 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 $(\mathbf{a}_i)^{\mathrm{T}}$ and $(\mathbf{a}_i^*)$. 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 $(\mathbf{a}_i)^{\mathrm{T}}$ be a conventional basis of the lattice $\mathbf{L}$ of the space group $\mathcal{G}$. With the relations (4.5), $k_i = q_i/N_i$, and $\mathbf{k} = \sum_{i=1}^{3} k_i \mathbf{a}_i^*$, equation (4.3) can be written

$$\boldsymbol{\Gamma}^{q_1 q_2 q_3}[(\boldsymbol{I},\boldsymbol{t})] = \boldsymbol{\Gamma}^{\mathbf{k}}[(\boldsymbol{I},\boldsymbol{t})] = \exp - i(\mathbf{k}\,\mathbf{t}). \tag{4.11}$$

Equation (4.11) has the same form if a primitive basis $(\mathbf{p}_i)^{\mathrm{T}}$ 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 $(\mathbf{p}_i)^{\mathrm{T}}$ 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 $\mid \mathbf{k} \mid \leq \mid \mathbf{K} - \mathbf{k} \mid$ 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.

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

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

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

$$\mathbf{k}' = \mathbf{k}\,\boldsymbol{W}^{-1} + \mathbf{K}, \quad \mathbf{K} \in \mathbf{L}^* \tag{4.12}$$

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 4.2.1) 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.*

$$\mathbf{k} = \mathbf{k}\,\boldsymbol{W} + \mathbf{K}, \quad \mathbf{K} \in \mathbf{L}^*, \tag{4.13}$$

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 4.2.2) 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 $\mathbf{\Gamma^k}(\mathcal{T})$ relative to $\mathcal{G}$ comprises all irreps $\mathbf{\Gamma^{k'}}(\mathcal{T})$ 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 $O(\mathbf{\Gamma^k}(\mathcal{T}))$ 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 3.1.1, 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* $\mathbf{\Phi}$. 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 $\mathbf{\Gamma^k}(\mathcal{T})$ 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 4.2.3) 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* $\mathbf{k}$.

4.3 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 $\mathsf{D}^{\mathbf{k},i}(\mathcal{G}^{\mathbf{k}})$ is an allowed irrep of $\mathcal{G}^{\mathbf{k}}$, then $\mathsf{D}^{\mathbf{k},i}(\boldsymbol{I}, \boldsymbol{t}) = \exp(-i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}$ holds. The matrix $\boldsymbol{I}$ is the identity matrix with $\dim(\boldsymbol{I}) = \dim(\mathsf{D}^{\mathbf{k},i}(\mathcal{G}^{\mathbf{k}}))$.

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 4.3.1 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:

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

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 3.2. The allowed irreps of $\mathcal{H}_0^{\mathbf{k}}$ are those whose matrices of the translation elements are of the form:

$$\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}(\boldsymbol{I},\boldsymbol{t}) = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}. \tag{4.14}$$

For self-conjugate irreps allowed irreps of $\mathcal{H}_0^{\mathbf{k}}$ yield allowed irreps of $\mathcal{G}^{\mathbf{k}}$, see equation 3.8 and 3.9.

For induction from non-self-conjugate irreps of $\mathcal{H}_0^{\mathbf{k}}$, see equations 3.6 and 3.7, the above result is also valid

$$(\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}(\boldsymbol{I},\boldsymbol{t}))_{(\boldsymbol{W},\boldsymbol{w})} = \mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}[(\boldsymbol{W},\boldsymbol{w})^{-1}(\boldsymbol{I},\boldsymbol{t})(\boldsymbol{W},\boldsymbol{w})] = \exp -(i\,(\mathbf{k}\,\boldsymbol{W}^{-1}\,\mathbf{t}))\,\boldsymbol{I} = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}, \tag{4.15}$$

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 $\mathcal{G}^{\mathbf{k}}$.

4.4 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 $\mathbf{D}^{\mathbf{k},i}$ of the corresponding little group $\mathcal{G}^{\mathbf{k}}$. If $\dim(\mathbf{D}^{\mathbf{k},i}) = r$ 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 $(\boldsymbol{W}_i,\,\boldsymbol{w}_i),\ \ i = 1,\ \ldots\ , s$ 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 4.3, 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 3.1.1. 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.

4.5 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. $\mathbf{k}$-vector information
   (a) Choice of a $\mathbf{k}$ vector (from the rep domain $\mathbf{\Phi}$ of the BZ). The coefficients of the $\mathbf{k}$ 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 $\mathbf{k}$:
   $\overline{\mathcal{G}}^{\mathbf{k}} = \{\, \widetilde{\boldsymbol{W}}_i \in \overline{\mathcal{G}} :\ \boldsymbol{k} = \boldsymbol{k}\, \widetilde{\boldsymbol{W}}_i + \boldsymbol{K},\ \mathbf{K} \in \mathbf{L}^*\}$
   (c) Determination of the $\mathbf{k}$-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 $\mathbf{D}^{\mathbf{k},\,i}$ of $\mathcal{G}^{\mathbf{k}}$ are related to the non-equivalent irreps $\overline{\mathbf{D}}^{\mathbf{k},\,i}$ of $\overline{\mathcal{G}}^{\mathbf{k}}$ in the following way:
   $\mathbf{D}^{\mathbf{k},\,i}(\, \widetilde{\boldsymbol{W}}_i,\, \widetilde{\boldsymbol{w}}_i) = \exp -(i\,\mathbf{k}\,\mathbf{w}_i)\, \overline{\mathbf{D}}^{\mathbf{k},\,i}(\, \widetilde{\boldsymbol{W}}_i)$
   (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 $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0}$ of $\mathcal{H}_0^{\mathbf{k}}$, *i. e.* those for which is fulfilled $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0}(\boldsymbol{I},\, \boldsymbol{t}) = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}$ 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 $\mathbf{D}^{\star\mathbf{k},i}$ of $\mathcal{G}$ from the allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}$
The representation matrices of $\mathbf{D}^{\star\mathbf{k},i}(\mathcal{G})$ 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 $\mathbf{D}^{\star\mathbf{k},m}$ of $\mathcal{G}$:

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

   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 $\mathbf{D}^{\mathbf{k},m}$ of the little group $\mathcal{G}^{\mathbf{k}}$ obtained in step 3.

4.6 Example 1. Irreps of *P4mm*, k vector X (0, 1/2, 0)

1. Space-group information

   (a) Decomposition of *P4mm* relative to its translation subgroup;
   coset representatives from IT A (1996)
   $(\boldsymbol{1}, \boldsymbol{o})$, $(\boldsymbol{2}_z,\, \boldsymbol{o})$, $(\boldsymbol{4}, \boldsymbol{o})$, $(\boldsymbol{4}^{-1},\, \boldsymbol{o})$, $(\boldsymbol{m}_{yz},\, \boldsymbol{o})$, $(\boldsymbol{m}_{xz},\, \boldsymbol{o})$, $(\boldsymbol{m}_{x\overline{x}},\, \boldsymbol{o})$, $(\boldsymbol{m}_{xx},\, \boldsymbol{o})$

   (b) generators of *P4mm* from IT A (1996)
   $\boldsymbol{t}_1,\ \boldsymbol{t}_2,\ \boldsymbol{t}_3,\ (\boldsymbol{2}_z,\, \boldsymbol{o}),\ (\boldsymbol{4}, \boldsymbol{o}),\ (\boldsymbol{m}_{yz},\, \boldsymbol{o})$

2. **k**-vector information

   (a) X (0, 1/2, 0)

(b) little co-group $\overline{\mathcal{G}}^X = \{\boldsymbol{1},\ \boldsymbol{2}_z,\ \boldsymbol{m}_{yz},\ \boldsymbol{m}_{xz}\} = 2_z m_{yz} m_{xz}$

$$e.g.,\ X\,2_z \ =\ (0,\,1/2,\,0)\begin{pmatrix} \overline{1} & 0 & 0 \\ 0 & \overline{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \ =\ (0,\,-1/2,\,0) \ =\ (0,\,1/2,\,0) + (0,\,\overline{1},\,0)$$

(c) **k**-vector star: $\star\, X = \{(0,\,1/2,\,0),\ (1/2,\,0,\,0)\}$
coset representative of $\overline{G} = 4mm$ relative to $\overline{G}^{\mathbf{k}} = 2_z m_{yz} m_{xz}$, HM symbol $mm2$
$4mm = 2_z m_{yz} m_{xz} \cup \boldsymbol{m}_{xx}\, 2_z m_{yz} m_{xz}$

(d) little group $\mathcal{G}^X = P2_z m_{yz} m_{xz}$, HM symbol $Pmm2$

(e) decomposition of $P4mm$ relative to $P2_z m_{yz} m_{xz}$
$P4mm = P2_z m_{yz} m_{xz} \cup (\boldsymbol{m}_{xx},\ \boldsymbol{o}) P2_z m_{yz} m_{xz}$

3. Allowed irreps of $\mathcal{G}^X$
Because $\mathcal{G}^X$ is a symmorphic group, $\mathbf{D}^{X,i}(\widetilde{W}_i,\ \widetilde{w}_i) = \exp -(i\,\mathbf{X}\,\widetilde{\mathbf{w}}_i)\,\overline{\mathbf{D}}^{X,i}(\widetilde{W}_i)$.
In the following table, $\boldsymbol{t}$ is the column of integer coefficients $(n_1,\ n_2,\ n_3)$

$P2_z mm$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{2}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz},\ \boldsymbol{o})$	$(\boldsymbol{m}_{xz},\ \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$
$\boldsymbol{D}^{X,1}$	1	1	1	1	$\exp -(i\,\mathbf{X}\,\mathbf{t})$
$\boldsymbol{D}^{X,2}$	1	1	-1	-1	$= \exp -(i\pi n_2)$
$\boldsymbol{D}^{X,3}$	1	-1	1	-1	$= (-1)^{n_2}$
$\boldsymbol{D}^{X,4}$	1	-1	-1	1	

4. Induction procedure
Generators of $P4mm$: $\langle(\boldsymbol{W}_l,\ \boldsymbol{w}_l)\rangle = \langle(\boldsymbol{1}, \boldsymbol{t}_i),\ (\boldsymbol{4}, \boldsymbol{o}),\ (\boldsymbol{m}_{yz},\ \boldsymbol{o})\rangle$
Representatives of $P2_z m_{yz} m_{xz}$ relative to $\mathcal{T}$:
$\{(\widetilde{W}_j,\ \widetilde{w}_j)\} = \{(\boldsymbol{1}, \boldsymbol{o}),\ (\boldsymbol{2}_z,\ \boldsymbol{o}), (\boldsymbol{m}_{yz},\ \boldsymbol{o}),\ (\boldsymbol{m}_{xz},\ \boldsymbol{o})\}$
Coset representatives of $P4mm$ relative to $P2_z m_{yz} m_{xz}$:
$\{q_1,\ q_2\} = \{(\boldsymbol{1}, \boldsymbol{o}),\ (\boldsymbol{m}_{xx},\ \boldsymbol{o})\}$.

(a) Induction matrix (for the group table of *4mm* see Table 3.1.1)

$(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}\,(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$	q_j	$q_i^{-1}\,(\boldsymbol{W}_l,\, \boldsymbol{w}_l)\,q_j$ $= (\widetilde{W}_j,\, \widetilde{w}_j)$	$M_{ij} \neq 0$
$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	1 1
	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{m}_{xx}\,\boldsymbol{t})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{m}_{xx}\,\boldsymbol{t})$	2 2
$(\boldsymbol{m}_{yz},\, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz},\, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz},\, \boldsymbol{o})$	1 1
	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{4}^{-1},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xz},\, \boldsymbol{o})$	2 2
$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{yz},\, \boldsymbol{o})$	1 2
	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xx},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xz},\, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz},\, \boldsymbol{o})$	2 1

(b) Matrices of the irreps $\mathbf{D}^{*X,i}$ of $\mathcal{G}$

$$\mathbf{D}^{*X,i}(\boldsymbol{1}, \boldsymbol{t}) = \left(\begin{array}{c|c} \mathbf{D}^{X,i}(\boldsymbol{1}, \boldsymbol{t}) & \boldsymbol{O} \\ \hline \boldsymbol{O} & \mathbf{D}^{X,i}(\boldsymbol{1}, \boldsymbol{m}_{xx}\boldsymbol{t}) \end{array}\right); \tag{4.16}$$

$$\mathbf{D}^{*X,i}(\boldsymbol{m}_{yz},\, \boldsymbol{o}) = \left(\begin{array}{c|c} \mathbf{D}^{X,i}(\boldsymbol{m}_{yz},\, \boldsymbol{o}) & \boldsymbol{O} \\ \hline \boldsymbol{O} & \mathbf{D}^{X,i}(\boldsymbol{m}_{xz},\, \boldsymbol{o}) \end{array}\right); \tag{4.17}$$

$$\mathbf{D}^{*X,i}(\boldsymbol{4}, \boldsymbol{o}) = \left(\begin{array}{c|c} \boldsymbol{O} & \mathbf{D}^{X,i}(\boldsymbol{m}_{yz},\, \boldsymbol{o}) \\ \hline \mathbf{D}^{X,i}(\boldsymbol{m}_{xz},\, \boldsymbol{o}) & \boldsymbol{O} \end{array}\right) \tag{4.18}$$

Table 4.6.1 Irreps $\mathbf{D}^{*X,\,i}$ for the generators of $P\bar{4}mm$ $\quad \boldsymbol{t} = (n_1,\ n_2,\ n_3)$

	$(\boldsymbol{m}_{yz},\ \boldsymbol{o})$	$(\bar{\boldsymbol{4}},\ \boldsymbol{o})$	$(\boldsymbol{1},\ \boldsymbol{t})$
$\mathbf{D}^{*X,\,1}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,\,2}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,\,3}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,\,4}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$

Chapter 5

Exercises, Problems

In this part the exercises of the School are presented. The necessary basic data: multiplication tables, matrices, character tables, *etc.* are listed in Chapter 6.

5.1 Exercise 1: Crystallographic groups

Problem 1
The 8 elements of the group *4mm* are represented by their matrices in Section 6.3.2. The multiplication table of the group *4mm* is displayed in Section 6.2.2.

Questions:

1. Which are the orders of the elements ?
2. How are these elements distributed into conjugacy classes ?
3. Which are the subgroups of *4mm* ? (use the mutiplication table).
4. Construct the complete subgroup diagram of point group *4mm*, see *Remark*. Which of these subgroups are conjugate (symmetrically equivalent) in *4mm* and which are normal subgroups?
5. Which composition series of *4mm* can be constructed from this list of subgroups? Compare the result with Fig. 1.2.1 on p. 11 and Table 1.2.2 on p. 12 of the manuscript.

Remark In a subgroup diagram each, subgroup is located at a level that is determined by its index (the original group with index [1] on top, subgroups of index [2] next lower level, etc.). Each of these groups is connected with its maximal subgroups by straight lines.

Problem 2
Show that any subgroup of index 2 is an invariant (normal) subgroup.

Problem 3
Consider the normal subgroup $\{e, 2\}$ of *4mm* of index 4. Determine the coset decomposition of *4mm* with respect to $\{e, 2\}$. Show that the cosets of the decomposition fulfill the group axioms and form a factor group. Determine the multiplication table of the factor group. Is the factor group isomorphic to some crystallographic point group?

Problem 4

The 'general position' of the space group *P4bm*, No. 100, is listed in *IT* A (*cf.* Fig. 6.2, page 60) as

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

Question:
Which matrix-column pairs or (4×4) matrices correspond to these 'coordinate triplets'?

Optional Exercise

Problem 5

The 6 elements of the group *3m* are represented by their matrices in Section 6.3.1. The multiplication table of the group *3m* is displayed in Section 6.2.1.

Questions:

1. Which are the orders of the elements ?
2. How are these elements distributed into conjugacy classes ?
3. Which are the subgroups of *3m* ? (use the mutiplication table).
4. Construct the complete subgroup diagram of point group *3m*. Which of these subgroups are conjugate (symmetrically equivalent) in *3m* and which are normal subgroups?
5. Which composition series of *3m* can be constructed from this list of subgroups? Compare the result with Fig. 1.2.2 on p. 11 and Table 1.2.3 on p. 13 of the manuscript.

Problem 6

Consider the group *4mm* and its subgroups of index 4. Determine the normalizers of these subgroups with respect to *4mm*.

5.2 Exercise 2: Irreducible representations of point groups

Problem 1

1. Derive the table of irreps for the groups $\mathcal{C}_3$ and $\mathcal{C}_4$ using lemma 2.2.1 on p. 17 of the manuscript.
2. Derive the table of irreps for the group $\mathcal{C}_6$:
   (a) using lemma 2.2.1 on p. 17 of the manuscript;
   (b) using the formula of Section 2.2.2 on p. 18 of the manuscript.

Problem 2

1. Derive the table of irreps for the group $4/m = 4 \times \overline{1}$.
2. What is the difference to the table of irreps for the group $4 \times m_z$?

Problem 3

1. Determine the number and the dimensions of the irreps of the group *4mm*. Calculate the character table of the group *4mm*.
2. Construct the character table of the group $\mathcal{D}_{4h}$ starting from the character table of $\mathcal{C}_{4v}$ and using the fact that $\mathcal{D}_{4h} = \mathcal{C}_{4v} \times \mathcal{C}_i$, where $\mathcal{C}_i$ is the group of inversion, $\mathcal{C}_i = \{\mathsf{e}, \overline{1}\}$.

Optional Exercise

Problem 4

Show that all irreps of Abelian groups are one-dimensional.

Problem 5

Determine the matrices of the representation of the group $\mathcal{C}_{4v}$ in the space of the five atomic d-orbitals: $\{d_{z^2} = z^2 f(r), d_{xy} = xyf(r), d_{yz} = yzf(r), d_{xz} = xzf(r), d_{x^2-y^2} = (x^2 - y^2)f(r)\}$ Here $f(r)$ is a function of r only. If the representation is reducible, determine the decomposition in irreps and the corresponding reduction matrix.

5.3 Exercise 3: Reducible and irreducible representations. Subduced and induced representations.

Problem 1

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. 6.1, page 59).
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. 6.2, page 60)?
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.

Problem 2
Consider the two-dimensional irrep $\mathbf{E}$ of point group *4mm* (see the first part of this exercise) 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 $\boldsymbol{S}^{-1}\,(\mathbf{E}\downarrow 4)(h)\,\boldsymbol{S} = \oplus m_i\,\mathbf{D}^i(h)$, $h \in 4$.

Problem 3

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.

Optional Exercises

Problem 4

Consider the two-dimensional irrep $\mathbf{E}$ of point group *4mm* (see the first part of this exercise) 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 $\boldsymbol{S}^{-1}\,(\mathbf{E}\downarrow mm2)(h)\,\boldsymbol{S} = \oplus m_i\,\mathbf{D}^i(h)$, $h \in mm2$.

Problem 5

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.

5.4 Exercise 4: Conjugate representations and orbits. Little groups and allowed irreps.

Problem 1

Using the character table of the group $\mathcal{C}_4$ and the multiplication table of the group $\mathcal{C}_{4v}$, distribute the irreps of the group $\mathcal{C}_4$ into orbits relative to $\mathcal{C}_{4v}$. For each of the irreps of $\mathcal{C}_4$ determine the corresponding little groups and allowed irreps.

Problem 2

Using the character table of the group $\mathcal{C}_{2v}$ and the multiplication table of the group $\mathcal{C}_{4v}$, distribute the irreps of the group $\mathcal{C}_{2v}$ into orbits relative to $\mathcal{C}_{4v}$. For each of the irreps of $\mathcal{C}_{2v}$ determine the corresponding little groups and allowed irreps.

Problem 3

Distribute the irreps of $\mathcal{D}_2$ into orbits relative to $\mathcal{T}$, using the character table of $\mathcal{D}_2$ and the multiplication table of $\mathcal{T}$ (*cf.* Section 6.2.3 for the multiplication table of $\mathcal{T}$).

Character table of $\mathcal{D}_2$

$\mathcal{D}_2$	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

Optional Exercise

Problem 4

Distribute the irreps of group *3* into orbits under conjugation of the group *3m*, using the multiplication table of *3m* and the character table of *3* from exercise 2.

5.5 Exercise 5: Derivation of the irreps of point groups by the induction procedure

Problem 1
By the 'induction procedure', derive the irreps of $\mathcal{D}_2$ from those of group $\mathcal{C}_2$ using the multiplication table for $\mathcal{D}_2$ and the table of irreps of $\mathcal{C}_2$.

Problem 2
By the 'induction procedure', derive the irreps of *4mm* from those of group *4* using the multiplication table for group *4mm* and the table of irreps of *4* (*cf.* Section 6.2.2 for the multiplication table of *4mm*).

Problem 3
By the 'induction procedure', derive (i) the irreps of the group $\mathcal{G} \times \overline{1}$ from those of the group $\mathcal{G}$; (ii) applying the results from (i) write down the irreps of $4/mmm$ starting from the irreps of $4mm$ obtained in Problem 2 above.

Optional exercises

Problem 4

By the 'induction procedure', derive the irreps of *3m* from those of group *3* using the multiplication table for *3m* (*cf.* Section 6.2.1 for the multiplication table of *3m*) and the table of irreps of *3* (Exercise 2).

Problem 5

Construct the irreps of group *23* by the 'induction procedure' starting from the irreps of *222* and the multiplication table of *23* (*cf.* Section 6.2.3 for the multiplication table of *23*).

Problem 6

By the 'induction procedure', derive the irreps of the 'quaternion group' $\mathcal{Q}_8$. The quaternion group is defined by the two generators a and b; the defining relations are

$$a^4 = e;\ b^2 = a^2;\ a\,b = b\,a^3.$$

Questions

1. Construct the multiplication table and the composition series of the group $\mathcal{Q}_8$;
2. Determine the number and dimensions of the irreps of the group $\mathcal{Q}_8$ and construct the irrep matrices by the 'induction procedure' starting from the irreps of the group $\mathcal{C}_4$, generated by a.

5.6 Exercise 6: Irreducible representations of space groups

Problem 1

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

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

Problem 2

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

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

Problem 3

Consider a general **k**-vector of a space group $\mathcal{G}$. Determine its little co-group, the **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 **k**-vector for a translation, $t \in \mathcal{T}_{\mathcal{G}}$.

Optional exercise

Problem 4

Consider the **k**-vectors $\Gamma(000)$ and $\mathbf{k} = \mathbf{R}\,(1/2,\,1/2,\,1/2)$ 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 $\Gamma(000)$ and $\mathbf{k} = \mathbf{R}\,(1/2,\,1/2,\,1/2)$;
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 $\Gamma(000)$ and $\mathbf{k} = \mathbf{R}\,(1/2,\,1/2,\,1/2)$, and construct the corresponding full space group irreps of $P2_13$.

Chapter 6

Appendix

The Appendix contains the necessary basic data for the exercises of Chapter 5: multiplication tables, matrices, character tables, *etc.* The first section repeats the induction procedure for the case of normal subgroups of index 2 or 3.

6.1 Special induction procedure for the determination of the irreps D of a group $\mathcal{G}$

Start from the irreps $\mathbf{D}^s$ 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: $q \in \mathcal{G}$ but $q \notin \mathcal{H}$
      i. $\mathcal{G} = \mathcal{H} \cup q\,\mathcal{H}$ for index 2
      ii. $\mathcal{G} = \mathcal{H} \cup q\,\mathcal{H} \cup q^2\,\mathcal{H}$ 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

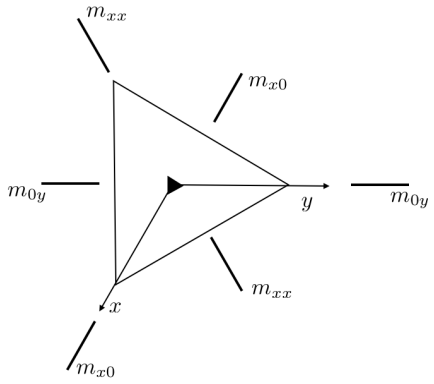
$$\boldsymbol{D}^s(q^{-1}\,h\,q) = \boldsymbol{U}^{-1}\,\boldsymbol{D}^s(h)\,\boldsymbol{U},\ h \in \mathcal{H}; \qquad \omega^3\,\boldsymbol{U}^3 = \boldsymbol{D}^s(q^3)$$

– $\{\mathbf{D}^s(\mathcal{H}), (\mathbf{D}^s(\mathcal{H}))q, (\mathbf{D}^s(\mathcal{H}))q^2\}$

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

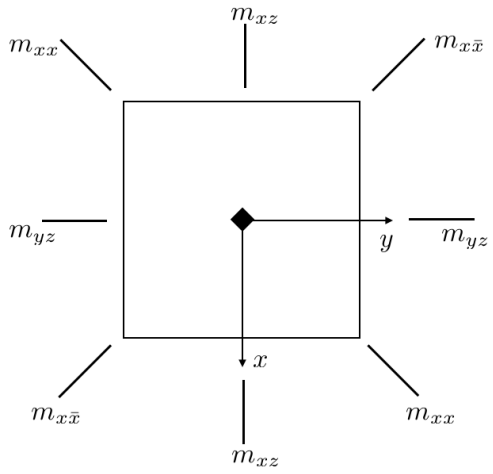
6.2 Multiplication (Cayley) tables

6.2.1 Symmetry elements and multiplication table of the group $3m$



$3m$	1	3_z	3_z^{-1}	m_{xx}	m_{x0}	m_{0y}
1	1	3_z	3_z^{-1}	m_{xx}	m_{x0}	m_{0y}
3_z	3_z	3_z^{-1}	1	m_{0y}	m_{xx}	m_{x0}
3_z^{-1}	3_z^{-1}	1	3_z	m_{x0}	m_{0y}	m_{xx}
m_{xx}	m_{xx}	m_{x0}	m_{0y}	1	3_z	3_z^{-1}
m_{x0}	m_{x0}	m_{0y}	m_{xx}	3_z^{-1}	1	3_z
m_{0y}	m_{0y}	m_{xx}	m_{x0}	3_z	3_z^{-1}	1

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



$4mm$	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\overline{x}}$
1	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\overline{x}}$
2_z	2_z	1	4_z^{-1}	4_z	m_{yz}	m_{xz}	$m_{x\overline{x}}$	m_{xx}
4_z	4_z	4_z^{-1}	2_z	1	m_{xx}	$m_{x\overline{x}}$	m_{yz}	m_{xz}
4_z^{-1}	4_z^{-1}	4_z	1	2_z	$m_{x\overline{x}}$	m_{xx}	m_{xz}	m_{yz}
m_{xz}	m_{xz}	m_{yz}	$m_{x\overline{x}}$	m_{xx}	1	2_z	4_z^{-1}	4_z
m_{yz}	m_{yz}	m_{xz}	m_{xx}	$m_{x\overline{x}}$	2_z	1	4_z	4_z^{-1}
m_{xx}	m_{xx}	$m_{x\overline{x}}$	m_{xz}	m_{yz}	4_z	4_z^{-1}	1	2_z
$m_{x\overline{x}}$	$m_{x\overline{x}}$	m_{xx}	m_{yz}	m_{xz}	4_z^{-1}	4_z	2_z	1

6.2.3 Multiplication table of the group $\mathcal{T}$

$\mathcal{T}$	e	a	b	c	q	r	s	t	q^2	r^2	s^2	t^2
e	e	a	b	c	q	r	s	t	q^2	r^2	s^2	t^2
a	a	e	c	b	t	s	r	q	s^2	t^2	q^2	r^2
b	b	c	e	a	r	q	t	s	t^2	s^2	r^2	q^2
c	c	b	a	e	s	t	q	r	r^2	q^2	t^2	s^2
q	q	s	t	r	q^2	s^2	t^2	r^2	e	b	c	a
r	r	t	s	q	t^2	r^2	q^2	s^2	b	e	a	c
s	s	q	r	t	r^2	t^2	s^2	q^2	c	a	e	b
t	t	r	q	s	s^2	q^2	r^2	t^2	a	c	b	e
q^2	q^2	t^2	r^2	s^2	e	c	a	b	q	t	r	s
r^2	r^2	s^2	q^2	t^2	c	e	b	a	s	r	t	q
s^2	s^2	r^2	t^2	q^2	a	b	e	c	t	q	s	r
t^2	t^2	q^2	s^2	r^2	b	a	c	e	r	s	q	t

6.3 Matrix groups; generating matrices

6.3.1 Matrices of the group *3m*

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

$$\boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \boldsymbol{m}_{x0} = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}; \boldsymbol{m}_{0y} = \begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix};$$

6.3.2 Matrices of the group *4mm*

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

$$\boldsymbol{m}_{yz} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \boldsymbol{m}_{xz} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \boldsymbol{m}_{x\overline{x}} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}; \boldsymbol{m}_{xx} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

6.4 Character tables

6.4.1 Character table of $\mathcal{D}_2$ (*222*)

$\mathcal{D}_2$	*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 $\mathcal{D}_3$ (*32*)

$\mathcal{D}_3$	1 (*1*)	2 (*3*)	3 (*2*)
$\mathbf{A}_1$	1	1	1
$\mathbf{A}_2$	1	1	−1
E	2	−1	0

6.4.2 Character table of *4*

4	*1*	*2*	*4*	4^3
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*)	1 (*2*)	2 (*4*)	2 (m_{xz})	2 (m_{xx})
$\mathbf{A}_1$	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

6.4.3 Character table of $\mathcal{T}$

The value of ϵ is $\exp 2\pi i/3$.

$\mathcal{T}$	$1\,(e)$	$3\,(a)$	$4\,(q)$	$4\,(q^2)$
A	1	1	1	1
^{1}**E**	1	1	ϵ	ϵ^*
^{2}**E**	1	1	ϵ^*	ϵ
T	3	-1	0	0

6.5 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 $\mathbf{k}$ vector (from the rep domain $\mathbf{\Phi}$ of the BZ). The coefficients of the $\mathbf{k}$ 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 $\mathbf{k}$:
   $\overline{\mathcal{G}}^{\mathbf{k}} = \{\,\widetilde{\boldsymbol{W}}_i \in \overline{\mathcal{G}} :\ \boldsymbol{k} = \boldsymbol{k}\,\widetilde{\boldsymbol{W}}_i + \boldsymbol{K},\ \mathbf{K} \in \mathbf{L}^*\}$
   (c) Determination of the $\mathbf{k}$-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 $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}^{\mathbf{k}}$ are related to the non-equivalent irreps $\overline{\mathbf{D}}^{\mathbf{k},i}$ of $\overline{\mathcal{G}}^{\mathbf{k}}$ in the following way:
$\mathbf{D}^{\mathbf{k},i}(\widetilde{\boldsymbol{W}}_i,\, \widetilde{\boldsymbol{w}}_i) = \exp -(i\,\mathbf{k}\,\mathbf{w}_i)\,\overline{\mathbf{D}}^{\mathbf{k},i}(\widetilde{\boldsymbol{W}}_i)$

(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 $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0}$ of $\mathcal{H}_0^{\mathbf{k}}$, *i. e.* those for which is fulfilled $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0}(\boldsymbol{I},\, \boldsymbol{t}) = \exp -(i\,\mathbf{k}\,\mathbf{t})\,\boldsymbol{I}$ 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 $\mathbf{D}^{\star\mathbf{k},i}$ of $\mathcal{G}$ from the allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}$
The representation matrices of $\mathbf{D}^{\star\mathbf{k},i}(\mathcal{G})$ 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}	$q_i^{-1}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)$	$q_i^{-1}(\boldsymbol{W}_l,\, \boldsymbol{w}_l)q_j$	$M(\boldsymbol{W}_l,\, \boldsymbol{w}_l)_{ij} \neq 0$
...	...	...	...	...	

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

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

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

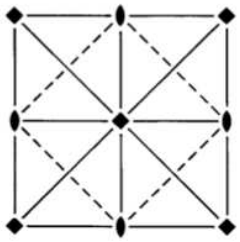
All irreps of the space group $\mathcal{G}$ for a given $\mathbf{k}$ vector are obtained considering all allowed irreps $\mathbf{D}^{\mathbf{k},m}$ of the little group $\mathcal{G}^{\mathbf{k}}$ obtained in step 3.

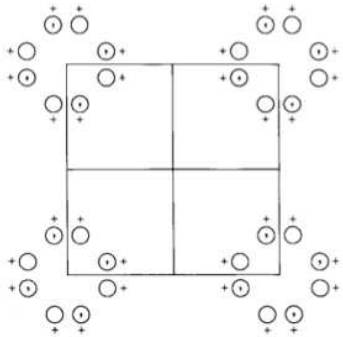
6.6 Space-group data

Figure 6.1: *IT*A space-group data for *P*4*mm* (selection)

*P*4*mm* C_{4v}^1 4*mm* Tetragonal

No. 99 *P*4*mm* Patterson symmetry *P*4/*mmm*





Origin on 4*mm*

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*

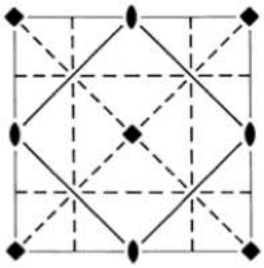
General position

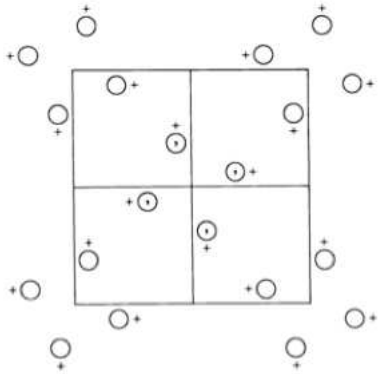
(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$
(5) $x,\bar{y},z$ (6) $\bar{x},y,z$ (7) $\bar{y},\bar{x},z$ (8) y,x,z

Figure 6.2: *IT*A space-group data for *P4bm* (selection)

P4bm C_{4v}^2 4*mm*

No. 100 *P4bm* 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

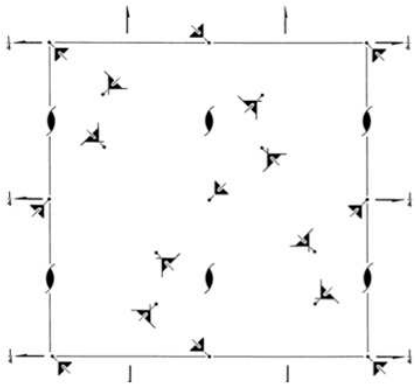
General position

(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 6.3: *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) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$

Part II

Online tools for representations of crystallographic groups on the Bilbao Crystallographic Server

Mois I. Aroyo

Departamento Física de la Materia Condensada
Universidad del País Vasco, Bilbao, Spain

Assen K. Kirov

Condensed Matter Physics Department, Sofia University,
BG-1486 Sofia, Bulgaria

J. Manuel Perez-Mato

Departamento Física de la Materia Condensada
Universidad del País Vasco, Bilbao, Spain

César Capillas

Departamento de Física de la Materia Condensada
Universidad del País Vasco, E-48080 Bilbao, Spain

Danel Orobengoa

Departamento Física de la Materia Condensada
Universidad del País Vasco, Bilbao, Spain

Gemma de la Flor

Departamento Física de la Materia Condensada
Universidad del País Vasco, Bilbao, Spain

Hans Wondratschek

Laboratorium für Applikationen der Synchrotronstrahlung (LAS)
Universität, Karlsruhe, Germany

Chapter 7

The Bilbao Crystallographic Server

The *Bilbao Crystallographic Server* is a web site with crystallographic databases and programs that can be used free of charge from any web browser via Internet. The server is on-line since 1998 and new programs are continuously added to the available tools. The server gives access to data in *International Tables for Crystallography, Volume A: Space group symmetry* (abbreviated as *IT*A) and data of maximal subgroups of plane and space groups as listed in *International Tables for Crystallography, Volume A*1: *Symmetry relations between space groups*. We have also started with the development of a database for subperiodic groups: the basic crystallographic data of the layer and rod groups (*International Tables for Crystallography, Volume E: Subperiodic groups* and their maximal subgroups are already accessible on the server.

The accompanying software is divided into several shells according to its complexity and proximity to the data contained in the database kernel. There are simple tools for retrieving data directly from the database such as generators and general positions, Wyckoff-position data and maximal subgroups. In addition, we have developed different applications which are essential for problems involving group-subgroup relations between space groups: subgroups and supergroups of space groups, graphs of maximal subgroups for an arbitrary group-subgroup pair, Wyckoff-position splitting schemes for group-subgroup pairs, *etc.* Detailed descriptions of the set of databases available on the server and the shell formed by the crystallographic computing programs (Aroyo *et al.*, 2006a).

In this Chapter we report on the databases and programs facilitating the application of representation theory to specific problems of solid-state physics and crystallography-related fields. The retrieval tool `POINT` gives access to a database with basic information on irreducible representations (abbreviated as irreps in the following) of crystallographic point groups like character tables, irrep multiplication tables, tables of tensor representations, *etc.*. The server includes also the so-called **k**-vector or Brilloiun-zone database. It consists of Brillouin-zone figures and tables for all 230 space groups of the wave-vectors symmetry types which are fundamental for the classification of the space-group irreps. The computing packages support certain essential (and more involved from a mathematical point of view) steps in the related group-theoretical studies. The server offers access to the basic modules for handling space-group representations

REPRES, it enables the study of the correlations between irreps of group-subgroup related space groups CORREL and the decomposition of Kronecker direct products of space-group irreps DIRPRO. In the following, the group-theoretical background of the developed programs are only briefly outlined (for more details the reader is referred to Aroyo *etc.*, 2006b). Illustrative examples explain the necessary input data and provide details on the output results.

7.1 Databases and retrieval tools

7.1.1 Point-group representations

The information about the 32 crystallographic point groups plays a fundamental role in many applications of crystallography. In the literature, there exists a lot of information about crystallographic point groups and their representations. Some complete tables are given in Koster *et al.* (1963), Bradley & Cracknell (1972), Altmann & Herzig (1994) (and the references therein). A selection of this data has been recalculated and it is now available online via the Bilbao Crystallographic Server. The point-group databases are part of the core shell of the server. The information about the irreps of the 32 point groups can be obtained from the program REPRES (*cf.* Section 7.2.1) for the particular case of $*\mathbf{k} = \Gamma(0,0,0)$. All generated point-group data has been stored as an XML database of the server. The retrieval tool POINT displays a set of several tables for each of the 32 crystallographic point groups which are specified by their international (Hermann-Mauguin) and Schoenflies symbols:

1. *Character table.* The character table provides the characters of the ordinary (vector) irreps of chosen point group. The irreps are labelled in the notation of Mullikan (1933) and by the Γ labels given by Koster *et al.* (1963). The matrices of the degenerate irreps as calculated by REPRES are also accessible. The number of point-group elements in a conjugacy class is indicated by the listed multiplicity. In addition, the transformation properties of the cartesian tensors of rank 1 (vectors and axial vectors) and 2 are displayed. (The tensor of rank 0 belongs always to the totally symmetric irrep and is not listed explicitly). Cartesian tensors that span two- or three-dimensional irreps are joined by brackets.

2. *Subgroup table.* The point-group types of the subgroups of a point group are listed with the corresponding indices in the initial point group.

3. *Irrep multiplication table.* The table shows the decomposition into irreducible constituents of the Kronecker (direct) product of any pair of point-group irreps.

4. *Tensor representations.* The table lists the decompositions into irreducible constituents of representations related to some important tensors (and their powers), such as the vector V (polar) or the pseudovector A (axial), their symmetrized $[V^2]$ or antisymmetrized squares, *etc.*

5. *Selection rules for fundamental transitions.* The table displays the selection rules for infrared and Raman electronic transitions. The data in the first row of each

table (specified by the trivial irrep label) corresponds to the usual infrared and Raman selection rules.

6. *Subduction from the rotation group irreps.* Given a (vector) representation of the rotation group of dimension $2l + 1$, $l = 0,\ldots,9$, the table lists the point-group irreps which appear in its subduction to the chosen point group.

7.1.2 k-vectors and Brillouin zones

The determination, classification, labeling and tabulation of irreducible representations (irreps) of space groups is based on the use of wave vectors **k**. The **k**-vector database available on the Bilbao Crystallographic Server contains figures of the Brillouin zones and tables which form the background of a classification of the irreps of all 230 space groups. In this compilation the symmetry properties of the wave vectors are described by the so-called *reciprocal-space groups* which are isomorphic to symmorphic space groups Wintgen, 1941, see also Aroyo and Wondratschek, 1995. This isomorphism allows the application of crystallographic conventions in the classification of the wave vectors (and henceforth in the irreps of the space groups). For example, the different symmetry types of **k**-vectors correspond to the different kinds of point orbits (Wyckoff positions) in the symmorphic space groups; the unit cells with the asymmetric units given in *IT*A can serve as Brillouin zones and representation domains, *etc.* The advantages of the reciprocal-space group approach compared to the traditional schemes of wave-vector classification can be summarized as follows:

- The asymmetric units given in *IT*A serve as representation domains which are independent of the different shapes of the Brillouin zones for different ratios of the lattice parameters.
- For the non-holohedral groups the representation domain is obtained from that of the corresponding holohedral group by extending the parameter ranges, not by introducing differently labeled special **k**-vector points, lines or planes of symmetry.
- A complete list of the special sites in the Brillouin zone is provided by the Wyckoff positions of *IT*A. The site symmetry of *IT*A corresponds to the little co-group of the wave vector; the number of branches of the star of **k** follows from the multiplicity of the Wyckoff position.
- All **k**-vector stars giving rise to the same type of irreps are related to the same Wyckoff position and designated by the same Wyckoff letter.

The available figures and the wave-vector data based on the reciprocal-space group symmetry are compared with the representation domains and the **k**-vector tables of the widespread tables of space-group representations by Cracknell, Davies, Miller and Love, 1979 (referred to as CDML).
The retrieval tool `KVEC` of the **k**-vector database uses as input the *IT*A-number of the space group. The output contains wave-vector tables and figures. There are several sets of figures and tables for the same space group when its Brillouin-zone shape

depends on the lattice parameters of the reciprocal lattice. The **k**-vector data are the same for space groups of the same arithmetic crystal class.

In the tables, the **k**-vector data as listed by CDML are compared with the Wyckoff-position description as given in *IT*A. Each **k**-vector type is specified by its label and parameters. The corresponding Wyckoff positions are described by their Wyckoff letters, multiplicities, and site symmetry groups. Their parameter description contains also the parameter ranges chosen in such a way that each orbit of the Wyckoff position of *IT*A, *i.e.* also each **k**-orbit, is listed *exactly once*. No ranges for the parameters are listed in CDML. Symmetry points, lines of symmetry or planes of CDML which are related to the same Wyckoff position are grouped together.

In the figures, the Brillouin zones of CDML and the conventional unit cells of *IT*A are displayed. The asymmetric units play the role of the representation domains of the Brillouin zones and they are chosen often in analogy to those of *IT*A. The names of **k**-vector points, lines, and planes of CDML are retained in this listing. New names have been given only to points and lines which are not listed in CDML.

Example: Brillouin zones and special k-vectors of the space group $F222$**.** The following example illustrates the relation between the traditional and the reciprocal-space group descriptions of the wave-vector types of space-group irreps. The included figures and tables form part of the output of the access tool `KVEC`.
The **k**-vector types of the space group $F222 \sim D_2^7$ are described with respect to the corresponding reciprocal space group which is isomorphic to $I222 \sim D_2^8$. Depending on the relations between the lattice constants *a, b* and *c*, there are two topologically different bodies of the Brillouin zone displayed in Fig. 7.1 and Fig. 7.2 by thin black lines; the first one has 24 vertices, 36 edges and 14 faces, the other has 18 vertices, 28 edges and 12 faces. The shape of the unit cell of *IT*A is always a parallelepipedon with 8 vertices, 12 edges and 6 faces. Similarly, the representation domains of CDML are more complicated than the asymmetric units of *IT*A, see Fig. 7.1 and Fig. 7.2.

The representatives of the **k**-vectors symmetry points or of symmetry lines, as well as the edges of the representation domain of CDML and of the chosen asymmetric unit are brought out in colors. A **k**-vectors symmetry point is designated by a red or cyan if it belongs to the asymmetric unit or to the representation domain of CDML. Points listed by CDML are not colored if they are part of a symmetry line or symmetry plane only. The color of the line is pink for an edge of the asymmetric unit which is not a symmetry line and it is red for a symmetry line of the asymmetric unit. The color of the line is brown with the name in red for a line which is a symmetry line as well as an edge of the asymmetric unit. The edges of the representation domains of CDML (displayed in the same figure) are colored in light blue. The corresponding symmetry points and lines are colored cyan. Edges of the representation domain or common edges of the representation domain and the asymmetric unit are colored dark blue with the letters in cyan if they are symmetry lines of the representation domain but not of the asymmetric unit.

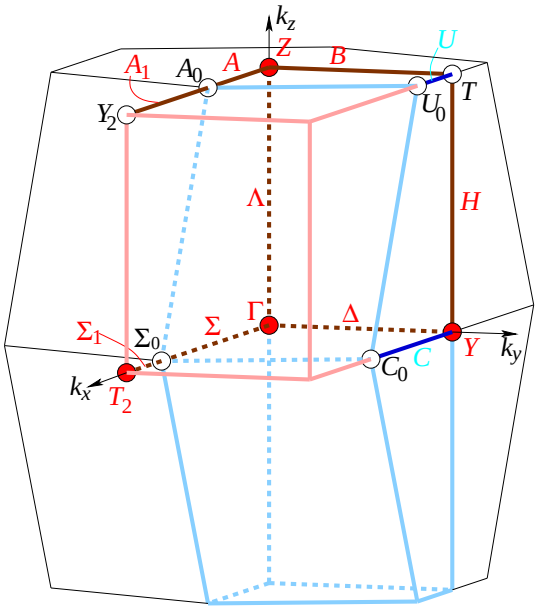


Figure 7.1: Brillouin zone and asymmetric unit and representation domain of CDML for the space group $F222 \sim D_2^7$: $a^{-2} < b^{-2} + c^{-2}, b^{-2} < c^{-2} + a^{-2}$and $c^{-2} < a^{-2} + b^{-2}$. Reciprocal-space group $I222^*$, No. 23. The representation domain of CDML is different from the asymmetric unit.

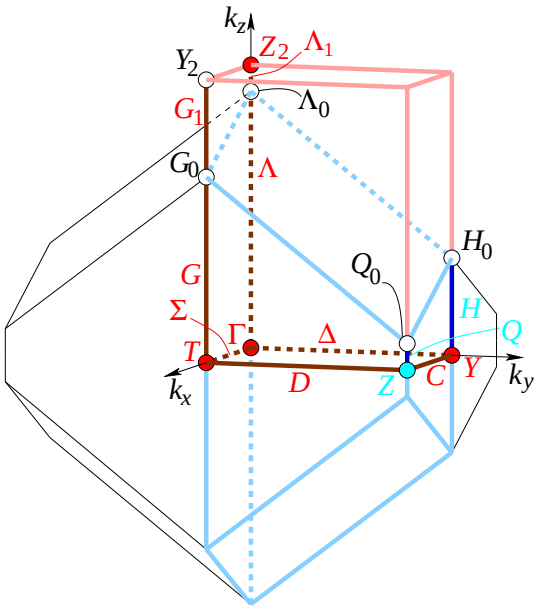


Figure 7.2: Brillouin zone and asymmetric unit and representation domain of CDML for the space group $F222 \sim D_2^7$: $c^{-2} > a^{-2} + b^{-2}$. Reciprocal-space group $I222^*$, No. 23. The representation domain of CDML is different from the asymmetric unit.

K-vector label			Wyckoff Position			ITA description
Primitive		Conventional-ITA	ITA			Coordinates
GM	0,0,0	0,0,0	a	2	222	0,0,0
T	1,1/2,1/2	0,1,1	b	2	222	0,1/2,1/2
$T\sim T_2$			b	2	222	1/2,0,0
Z	1/2,1/2 ,0	0,0,1	c	2	222	0,0,1/2
Y	1/2, 0, 1/2	0,1,0	d	2	222	0,1/2,0
$Y\sim Y_2$			d	2	222	1/2,0,1/2
SM	0, u, u ex	2u,0,0	e	4	2..	$x,0,0 : 0 < x <= sm_0$
U	1, 1/2+u, 1/2+u ex	2u,1,1	e	4	2..	$x,1/2,1/2 : 0 < x < u_0$
$U\sim SM_1=[SM_0\ T_2]$			e	4	2..	$x,0,0 : 1/2-u_0=sm_0 < x < 1/2$
$SM+SM_1=[GM\ T_2]$			e	4	2..	$x,0,0 : 0 < x < 1/2$
A	1/2, 1/2+u, u ex	2u,0,1	f	4	2..	$x,0,1/2 : 0 < x <= a_0$
C	1/2, u, 1/2+u ex	2u,1,0	f	4	2..	$x,1/2,0 : 0 < x < c_0$
$C\sim A_1=[A_0\ Y_2]$			f	4	2..	$x,0,1/2 : 1/2-c_0=a_0 < x < 1/2$
$A+A_1=[Z\ Y_2]$			f	4	2..	$x,0,1/2 : 0 < x < 1/2$

Figure 7.3: List of **k**-vector types (selection) for the space group $F222 \sim D_2^7$: $a^{-2} < b^{-2} + c^{-2}, b^{-2} < c^{-2}+a^{-2}$and $c^{-2} < a^{-2}+b^{-2}$. Reciprocal-space group $I222^*$, No. 23 (*cf* Fig. 7.1).

To save space we have included only part of the list of **k**-vector relations for the space group $F222 \sim D_2^7$ in the table shown in Fig. 7.3 (a screen-shot of the output of the access tool `KVEC`), corresponding to Fig. 7.1. The **k**-vector parameters of CDML (second column) of the table in Fig. 7.3 are different from those of *IT*A (last column) because in CDML the data are always referred to a primitive basis, whereas in *IT*A they are referred to a centered basis if appropriate, *e. g.* in F and I lattices. The coefficients of the **k**-vectors with respect to the basis that is dual to the conventional (centred) setting used in *IT*A, are listed under the 'Conventional ITA' column. The parameter ranges (last column) are chosen such that each **k**-vector orbit is represented exactly once.

One takes from the table given in Fig. 7.3 that different **k** labels of CDML (first column) may belong to the same type of **k** vectors, *i. e.* they give rise to the same type of irreps. Due to the special shape of the representation domain of CDML the special wave-vector line corresponding to the Wyckoff position 4 f 2.. (fourth column) is split into two parts, A and C. In the *IT*A description $A \cup C$ corresponds to one line $[ZY_2]$, $(x,\ 0,\ \frac{1}{2})$, with $0 < x < \frac{1}{2}$. The splitting of the 4 f line into two parts is a consequence of the Brillouin-zone shape for the specific values of the lattice parameters. This is confirmed from Fig. 7.2 where the corresponding special line C is not split.

7.2 Representations of space groups

There exist several reference sets of tables of space-groups irreps (see *e.g.* CDML, and the references therein). However, the available data have important drawbacks related to the lack of full space-group representations due to the limitations and/or specificity in the choice of the **k**-vectors. In addition, the used space-group settings

are often not compatible with those of *IT*A. These disadvantages are overcome by the program REPRES which computes the irreps of space groups explicitly: For any space group $\mathcal{G}$ and a $\mathbf{k}$-vector, the corresponding little group $\mathcal{G}^{\mathbf{k}}$, the allowed (little-group) irreps and the matrices of the full-group irreps are constructed. As part of the working environment of the Bilbao Crystallographic server, the program REPRES provides the irrep data in a format suitable for its further use as input for other programs on the server.
REPRES calculates the irreps of space groups following the algorithm based on a normal-subgroup induction method of constructing the irreps of a group $\mathcal{G}$ starting from those of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$. The main steps of the procedure involve the construction of all irreps of $\mathcal{H}$ and their distribution into orbits under $\mathcal{G}$, determination of the corresponding little groups and the allowed (small) irreps and finally, construction of the irreps of $\mathcal{G}$ by induction from the allowed irreps.

The application of the general normal-subgroup induction procedure in the case of space groups is straightforward. A normal subgroup of every space group is its *translation group* $\mathcal{T}$. The irreps of $\mathcal{T}$ are well-known and their distribution into orbits, the determination of the related little groups and the induction of the space-group irreps follow closely the general scheme. The most involved step in the procedure is the determination of the allowed irreps of the little group. These are calculated in REPRES using 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.

7.2.1 The program REPRES

Input Information

- Space group data: As an input the program needs the specification of the space group $\mathcal{G}$ which can be defined by its sequential *IT*A number. Here, as well as in the rest of programs related to space-group representations, the following *IT*A conventional settings are chosen as default: *unique axis b* setting for monoclinic groups, *hexagonal axes* setting for rhombohedral groups, and *origin choice 2* for the centrosymmetric groups listed with respect to two origins in *IT*A. The program REPRES can treat space groups in unconventional settings, once the transformation matrix-column pair $(\boldsymbol{P}, \boldsymbol{p})$ to the corresponding conventional setting is known. The 3×3 square matrix $\boldsymbol{P} = \| P_{ij} \|$ transforms the conventional basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ of $\mathcal{G}$ to the non-conventional $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ one:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}. \tag{7.1}$$

  The column $\boldsymbol{p} = (p_1, p_2, p_3)$ of coordinates of the non-conventional origin O' is referred to the conventional coordinate system of $\mathcal{G}$.

- $\mathbf{k}$-vector data: The $\mathbf{k}$-vector data can be introduced in two different ways: either by choosing the $\mathbf{k}$-vector directly from a table, or by keying in the $\mathbf{k}$-vector

coefficients from which the program identifies and assigns the corresponding **k**-vector label according to the classification scheme of CDML. This label is used to designate the irreps of the little and space groups. The program accepts **k**-vector coefficients given with respect to different coordinate systems of the reciprocal space. For its internal calculations `REPRES` uses **k**-vector coefficients (k_1, k_2, k_3) referred to a basis $(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)$ which is dual to the conventional *IT*A settings of the space groups (called *conventional* **k**-vector coefficients). The program accepts also **k**-vector coefficients referred to a primitive basis $(\mathbf{p_1^*}, \mathbf{p_2^*}, \mathbf{p_3^*})$ of the reciprocal lattice as given for example, in CDML tables of space-group irreps. The relation between the conventional and primitive **k**-vector coefficientsindex are given in Table 7.1.2. If a non-conventional setting for the space group is chosen (7.1), then the corresponding 'non-conventional' **k**-vector coefficients

$$(k_1', k_2', k_3') = (k_1, k_2, k_3)\boldsymbol{P}, \tag{7.2}$$

can be given as input data. Note that the program does not accept variables (free parameters) as coefficients of the wave vector.

The Brillouin-zones database with wave-vector tables for all 230 space groups and figures of the Brilloiun zones is available on the Bilbao Crystallographic server.

Output Information

The output produced by `REPRES` contains the following data:

1. Information on the space group $\mathcal{G}$:
   - non-translational generators of $\mathcal{G}$ listed as matrix-column pairs ($\boldsymbol{W}$,$\boldsymbol{w}$), *i.e.* in (3×4) matrix form. The sequence of generators follows that of *IT*A for the conventional settings of the space groups;
   - list of translational coset representatives ($\boldsymbol{W}$,$\boldsymbol{w}$) of $\mathcal{G}$, given in (3×4) matrix form. The numbers coincide with the sequential numbers of the general-position coordinate triplets listed in *IT*A.
2. **k**-vector data: The program lists the input values of the **k**-vector coefficients followed by the corresponding conventional coefficients (k_1, k_2, k_3). The coefficients of the arms of the wave-vector star $\mathbf{*k}$ are referred also to the basis that is dual to the conventional (default) setting of the space group.
3. Information on the little group $\mathcal{G}^{\mathbf{k}}$:
   - a set of coset representatives of $\mathcal{G}$ with respect to the little group $\mathcal{G}^{\mathbf{k}}$;
   - a set of non-translational generators and a set of translational coset representatives of $\mathcal{G}^{\mathbf{k}}$ given as (3x4) matrices;
   - little-group irreps presented in a matrix form for the translational coset representatives of $\mathcal{G}^{\mathbf{k}}$ in a consecutive order. The little-group irreps are labeled following the convention of CDML.

4. Full-group representations: The block of the full-group irreps starts with a list of the characters of the full-group irreps for all translational coset representatives of $\mathcal{G}$ followed by a list of the *physically irreducible representations*. (If an irrep is complex and not equivalent to any real irreducible representation, then the physically irreducible representation is formed by the direct sum of the irrep and its complex conjugate. Such representations are designated by two irrep symbols that follow each other. If an irrep is real, or equivalent to a real one, then the physically irreducible representation coincides with the irrep and the symbol of the physically irreducible representation corresponds to that of the irrep.)

   Optionally, the program gives also the full group irreducible representations of the non-translational generators of the space group in a block-matrix form: for a given representation and a generator, the program prints out the induction matrix whose non-zero entries, specified by its row and column indices, indicate a matrix block corresponding to a little-group matrix.

Example: Irreps of *P4bm* for $\mathbf{k} = \mathbf{X}(0, 1/2, 0)$

The **INPUT** data consists in the specification of the space group *P4bm* by its *IT*A number, No.100, and the data for **k**-vector coefficients, $\mathbf{k} = \mathbf{X}(0, 1/2, 0)$. (In all space groups with primitive lattices, the **k**-vector coefficients (k_{p1}, k_{p2}, k_{p3}), referred to a primitive basis of the reciprocal space (CDML), coincide with the conventional **k**-vector coefficients, *cf.* Table 7.1.2.)
The discussion of the **OUTPUT** follows the order of the results as they appear in the output file. All space-group elements $(\boldsymbol{W}, \boldsymbol{w})$ are given in a matrix-column form consisting of a (3×3) matrix part $\boldsymbol{W}$ and a (3×1)-column part $\boldsymbol{w}$:

$$(\boldsymbol{W}, \boldsymbol{w}) = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \end{pmatrix};$$

1. The *Space-group information* block contains the following data:
   (a) The generators of *P4bm* (with the exception of the generating translations) are listed in the same sequence as they appear in *IT*A: $(\boldsymbol{1}, \boldsymbol{o})$, $(\boldsymbol{2}_z, \boldsymbol{o})$, $(\boldsymbol{4}_z, \boldsymbol{o})$, $(\boldsymbol{m}_{yz}, \tau)$, with $\tau = (1/2, 1/2, 0)$[1].
   (b) Decomposition of *P4bm* relative to its translation subgroup with coset representatives as given in *IT*A: $(\boldsymbol{1}, \boldsymbol{o})$, $(\boldsymbol{2}_z, \boldsymbol{o})$, $(\boldsymbol{4}_z, \boldsymbol{o})$, $(\boldsymbol{4}_z^3, \boldsymbol{o})$, $(\boldsymbol{m}_{yz}, \tau)$, $(\boldsymbol{m}_{xz}, \tau)$, $(\boldsymbol{m}_{x\overline{x}}, \tau)$, $(\boldsymbol{m}_{xx}, \tau)$.
2. **k**-*vector information* block gives the information on:
   (a) The input **k**-vector coefficients **X**(0, 1/2, 0) followed by the corresponding conventional coefficients.
   (b) The **k**-vector star: $*\mathbf{X} = \{(0, 1/2, 0), (1/2, 0, 0)\}$.

[1] To make the description more compact we use a symbolic notation for the space-group elements.

(c) The little group $\mathcal{G}^{\mathbf{X}} = P2_zba$ is specified by the coset representatives of its decomposition with respect to the translation subgroup: $(\boldsymbol{1}, \boldsymbol{o})$, $(\boldsymbol{2}_z, \boldsymbol{o})$, $(\boldsymbol{m}_{xz}, \tau)$, $(\boldsymbol{m}_{yz}, \tau)$. The little co-group $\overline{\mathcal{G}}^{\mathbf{X}} = \{\boldsymbol{1}, \boldsymbol{2}_z, \boldsymbol{m}_{yz}, \boldsymbol{m}_{xz}\}$ is isomorphic to the point group 2_zmm.

(d) The coset representatives of the decomposition of $P4bm$ relative to $P2_zba$ $P4bm = P2_zba + (\boldsymbol{4}_z, \boldsymbol{o})P2_zba$

3. *Allowed irreps of* $\mathcal{G}^{\mathbf{X}}$

As the little group $\mathcal{G}^{\mathbf{X}}$ is non-symmorphic and the $\mathbf{k}$ vector is on the surface of the Brillouin zone, it is not possible to relate directly the allowed irreps of $P2_zba$ with the linear irreps of the little co-group $2mm$. The program determines the allowed irreps by constructing the composition series for the little group $P2_zba$:

$$P2_zba \rhd P2_z \rhd \mathcal{T}$$

The allowed irreps of $P2_zba$ are obtained in two steps:

(a) Construction of the allowed irreps of $P2_z$ starting from those of the translational subgroup $\mathcal{T}$:

$P2_z$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{2}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$
$\boldsymbol{D}^{\mathbf{X},1}_{P2_z}$	1	1	$\exp -(i\pi n_2)$
$\boldsymbol{D}^{\mathbf{X},2}_{P2_z}$	1	-1	$\exp -(i\pi n_2)$

Here, $\boldsymbol{t}$ is the column of coefficients (n_1, n_2, n_3).

(b) From the conjugation of the elements of $P2_z$ under $(\boldsymbol{m}_{yz}, \tau)$ follows that the two allowed irreps of $P2_z$ form an orbit of conjugate irreps, *i*.e. there is just one allowed two-dimensional irrep of $P2_zba$.

$P2_zba$	$(\boldsymbol{2}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \tau)$	$(\boldsymbol{m}_{xz}, \tau)$
$\boldsymbol{D}^{\mathbf{X},1}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

The program lists the corresponding irrep matrices following the consecutive order of the translational coset representatives of the little group. The (complex) matrix elements are specified by their moduli and phase angles in degrees [$\circ$]. For example, the matrix of the element $(\boldsymbol{m}_{yz}, \tau)$, listed under No.4, has the form:

$$\begin{pmatrix} (0.000, & 0.0) & (1.000, & 180.0) \\ (1.000, & 0.0) & (0.000, & 0.0) \end{pmatrix}.$$

4. *Full-group irreps* The full-group irrep $*\mathbf{X}, 1$ coincides with the physically irreducible representation, and its characters for all translation coset representatives of $P4bm$ are listed at the beginning of the full-group irrep block. In addition, the matrices of the full-group irreps for the non-translation generators are presented in a block-matrix form. The program lists separately the induction matrix $\boldsymbol{M}(\boldsymbol{W}, \boldsymbol{w})$ and the corresponding blocks of the little-group representation matrices specified by the row-column indices of the non-zero entries of $\boldsymbol{M}(\boldsymbol{W}, \boldsymbol{w})$. For example, the matrix of the full-group irrep for the generator $(\boldsymbol{4}_z, \boldsymbol{o})$ of $P4bm$ (No.3 in the list of generators)

$$\boldsymbol{D}^{*\mathbf{X},1}(\boldsymbol{4}_z,\, \boldsymbol{o}) \;=\; \left(\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \overline{1} \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right)$$

is presented as a (2×2) induction matrix

$$\boldsymbol{M}^{*\mathbf{X},1}(\boldsymbol{4}_z,\, \boldsymbol{o}) \;=\; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

with the following (2×2) blocks:

$$\text{Block (1,2)} \;=\; \begin{pmatrix} (1.000,\, 0.0) & (0.000,\, 0.0) \\ (0.000,\, 0.0) & (1.000,\, 180.0) \end{pmatrix};$$
$$\text{Block (2,1)} \;=\; \begin{pmatrix} (1.000,\, 0.0) & (0.000,\, 0.0) \\ (0.000,\, 0.0) & (1.000,\, 0.0) \end{pmatrix}.$$

7.3 Correlations between the representations of group-subgroup related space groups

7.3.1 The problem

For different physical applications it is important to know the *compatibility relations* (known also as *correlations*) between the representations of group-subgroup related crystallographic groups $\mathcal{H} < \mathcal{G}$. For their calculation it is sufficient to consider the irreps of $\mathcal{G}$. The problem can be formulated as follows: Given an irrep $\boldsymbol{D}_\mathcal{G}$ of $\mathcal{G}$, how does the subduced representation $\boldsymbol{D}^s_\mathcal{G} = \boldsymbol{D}_\mathcal{G} \downarrow \mathcal{H}$ decompose into irreps of $\boldsymbol{D}_\mathcal{H}$ of $\mathcal{H}$? This subduced representation $\boldsymbol{D}^s_\mathcal{G}$ is in general a reducible one and can be transformed into a direct sum of irreps $\boldsymbol{D}_\mathcal{H}$ of $\mathcal{H}$ by a suitable unitary transformation $\boldsymbol{S}$:

$$\boldsymbol{D}^s_\mathcal{G}\boldsymbol{S} = \boldsymbol{S}[\oplus \boldsymbol{E}(s \mid i) \otimes \boldsymbol{D}^i_\mathcal{H}], \tag{7.3}$$

where $\boldsymbol{E}(s \mid i)$ is the unit matrix of dimension $(s \mid i)$, and $(s \mid i)$ is the number of times the irrep $\boldsymbol{D}^i_{\mathcal{H}}$ is contained in the $\boldsymbol{D}^S_{\mathcal{G}}$ (the so-called *subduction coefficients*). The matrix $\boldsymbol{S}$ is known as the *subduction matrix*.
The problem of subduction coefficients and subduction matrices for crystallographic point groups is completely solved. For example, data on subduction coefficients for the irreps of point groups has been tabulated long ago (Koster *et al.*, 1963). However, similar results on subduction quantities for crystallographic space groups are only partially known. The difficulties in their tabulation are related to the great number and variety of space-group representations and possible group-subgroup relations between space groups.
The software package `CORREL` computes the CORRELations between representations of a crystallographic space group $\mathcal{G}$ and those of its subgroups $\mathcal{H}$, including the multiplicities of $\boldsymbol{D}^i_{\mathcal{H}}$ in $\boldsymbol{D}_{\mathcal{G}} \downarrow \mathcal{H}$. The module of the program for the determination of the subduction matrices $\boldsymbol{S}$ which relate the bases of the irreducible constituents $\boldsymbol{D}^i_{\mathcal{H}}$ to those of the subduced representation $\boldsymbol{D}_{\mathcal{G}} \downarrow \mathcal{H}$, Equ. (7.3), is still under development and for the moment the calculation of $\boldsymbol{S}$ is only optional.

7.3.2 The method

The space-group formulation of the subduction problem is straightforward. The subduced representation $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i} \downarrow \mathcal{H}$ is in general a reducible one and can be transformed into a direct sum of irreps $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ of $\mathcal{H}$ by a suitable transformation $\boldsymbol{S}$:

$$(\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i} \downarrow \mathcal{H})\boldsymbol{S} = \boldsymbol{S}[\oplus \boldsymbol{E}(*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j) \otimes \boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}]. \tag{7.4}$$

The direct sum is over all stars $*\mathbf{k}_{\mathcal{H}}$ of $\mathcal{H}$, and over all allowable irreps $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ which may arise for a given $*\mathbf{k}_{\mathcal{H}}$. The subduction coefficients $(*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j)$ are integers and denote the multiplicity of irreps $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ in the subduced representation. The rows of the subduction matrix $\boldsymbol{S}$ are labeled by the row-indices of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i}$. The columns of the subduction matrix are specified by a triple of indices indicating the irrep $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$, its multiplicity and a row index. The coefficients of a given column of $\boldsymbol{S}$ determine the linear combination of the basis functions of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i}$ that transforms as the corresponding row of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$.
We are interested in the calculation of the subduction coefficients and the subduction matrix $\boldsymbol{S}$.

In order to determine the subduction coefficients $(*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j)$ one can proceed by rewriting the defining equation (7.4) using the character systems $\chi^{*\mathbf{k}_{\mathcal{G}},i}$ of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i}$ and $\chi^{*\mathbf{k}_{\mathcal{H}},j}$ of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$:

$$\chi^{*\mathbf{k}_{\mathcal{G}},i}(h) = \sum (*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j)\chi^{*\mathbf{k}_{\mathcal{H}},j}(h), h \in \mathcal{H}. \tag{7.5}$$

The application of the orthogonality properties of the characters of the irreps $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ to Equ. (7.5) results in an expression for the subduction coefficients that is difficult to use directly: it would involve a sum over all elements of the subgroup. An alternative to the conventional routine for determination of $(*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j)$ follows directly from their definition. Although the sum in Equ. (7.4) is over all stars $*\mathbf{k}_{\mathcal{H}}$, in fact only

representations from a small number of stars are contained in the subduced representation. The determination of the splitting of the star $*\mathbf{k}_{\mathcal{G}}$ of $\mathcal{G}$ into stars $*\mathbf{k}_{\mathcal{H}}$ of $\mathcal{H}$ is the first step in the procedure for the determination of the subduction coefficients. Due to the decomposability of the subduced representations into irreducible constituents (7.4) the star $*\mathbf{k}_{\mathcal{G}}$ is decomposed into entire stars $*\mathbf{k}_{\mathcal{H}}$. One can formally introduce ***k**-*subduction coefficients* $(*\mathbf{k}_{\mathcal{G}} \mid *\mathbf{k}_{\mathcal{H}})$ to describe the splitting of the star $*\mathbf{k}_{\mathcal{G}}$:

$$*\mathbf{k}_{\mathcal{G}} = \sum_{*\mathbf{k}_{\mathcal{H}}} (*\mathbf{k}_{\mathcal{G}} \mid *\mathbf{k}_{\mathcal{H}}) *\mathbf{k}_{\mathcal{H}}, \tag{7.6}$$

where the sum is over the stars $*\mathbf{k}_{\mathcal{H}}$ that occur in $*\mathbf{k}_{\mathcal{G}}$. The coefficients $(*\mathbf{k}_{\mathcal{G}} \mid *\mathbf{k}_{\mathcal{H}})$ are integers and they relate in an obvious way the number of arms $s_{\mathbf{k}_{\mathcal{G}}}$ and $s_{\mathbf{k}_{\mathcal{H}}}$ of the stars $*\mathbf{k}_{\mathcal{G}}$ and $*\mathbf{k}_{\mathcal{H}}$:

$$s_{\mathbf{k}_{\mathcal{G}}} = \sum (*\mathbf{k}_{\mathcal{G}} \mid *\mathbf{k}_{\mathcal{H}}) s_{\mathbf{k}_{\mathcal{H}}} \ . \tag{7.7}$$

The ***k**-*subduction coefficients* are determined by direct inspection: starting from an arbitrary arm of $*\mathbf{k}_{\mathcal{G}}$ one determines all those arms $\mathbf{k}_{\mathcal{G}}$ which belong to the corresponding star $*\mathbf{k}_{\mathcal{H}}$. If any vectors $\mathbf{k}_{\mathcal{G}}$ are left one continues with the procedure until all $*\mathbf{k}_{\mathcal{G}}$ arms are distributed into $*\mathbf{k}_{\mathcal{H}}$ stars.

The determination of the ***k**-*subduction coefficients* reduces the sum in Equ. (7.5), and in this way simplifies the calculation of the subduction coefficients. Consider a star $*\mathbf{k}_{\mathcal{H}}$ with $(*\mathbf{k}_{\mathcal{G}} \mid *\mathbf{k}_{\mathcal{H}}) \neq 0$ whose $n_{\mathbf{k}_{\mathcal{H}}}$ irreps are of dimensions $d^{*\mathbf{k}_{\mathcal{H}},j} = \dim(\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j})$. A set of linear algebraic equations with the subduction coefficients as unknowns is obtained taking Equs. (7.5) for different elements of $\mathcal{H}$. Their number equals $\sum n_{\mathbf{k}_{\mathcal{H}}}$, where the sum is over the number of distinct $*\mathbf{k}_{\mathcal{H}}$ stars that occur in $*\mathbf{k}_{\mathcal{G}}$.

Once the subduction coefficients are determined it is possible to construct the block-diagonal representation $\oplus \boldsymbol{E}(*\mathbf{k}_{\mathcal{G}}, i \mid *\mathbf{k}_{\mathcal{H}}, j) \otimes \boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$, equivalent to the subduced representation $(\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i} \downarrow \mathcal{H})$. The set of matrix equations (7.4) for the elements of $\mathcal{H}$ forms a system of linear equations with the elements of the subduction matrix $\boldsymbol{S}$ as unknowns. For the explicit calculation of the elements of the subduction matrix it is convenient to split and rewrite Equ. (7.4) for each $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ separately:

$$(\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i} \downarrow \mathcal{H}) \boldsymbol{S}^{*\mathbf{k}_{\mathcal{H}},j} = \boldsymbol{S}^{*\mathbf{k}_{\mathcal{H}},j} \boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j} \ . \tag{7.8}$$

Here the rectangular matrices $\boldsymbol{S}^{*\mathbf{k}_{\mathcal{H}},j}$ consist of $d^{*\mathbf{k}_{\mathcal{H}},j}$ columns of $\boldsymbol{S}$ and correspond to the elements of the subduction matrix associated with the irrep $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$. The number of independent solutions of (7.8) equals the multiplicity of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ in the subduced representation. One should note that: (i) we are interested only in the nonsingular solutions for the subduction matrix, and (ii) the freedom in the determination of $\boldsymbol{S}$ follows from the Schur lemma for reducible representations: the subduction matrix $\boldsymbol{S}$ is determined up to a matrix belonging to the commuting algebra of the representation $\oplus \boldsymbol{E}(*\mathbf{k}_{\mathcal{G}}, i \mid *\mathbf{k}_{\mathcal{H}}, j) \otimes \boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$.

7.3.3 The program CORREL

As **Input** data the program requires the groups $\mathcal{G}$ and $\mathcal{H}$ specified by their *IT*A-numbers, and a transformation matrix-column pair ($\boldsymbol{P}$, $\boldsymbol{p}$) relating the conventional (default) bases of the group and the subgroup, Equ. (7.1). The **k**-vector coefficients could be referred to the primitive bases of reciprocal space (of the supergroup) as found in CDML. Another possibility for the cases of centered lattices is to refer the **k**-vector to the centered basis dual to the conventional setting of the space group, *i.e.* the conventional **k**-vector coefficients (*cf.* Section 7.2.1).

The **Output** consists of five main subblocks. The listed data starts with information on the studied group-subgroup pair of space groups $\mathcal{G} > \mathcal{H}$ including their space group numbers and lattice types, lists of generators and translational coset representatives ($\boldsymbol{W}, \boldsymbol{w}$) given in ($3 \times 4$) matrix form, and the transformation matrix-column pair ($\boldsymbol{P}, \boldsymbol{p}$). The $*\mathbf{k}_{\mathcal{G}}$ vector is specified by its input coefficients and those referred to the dual basis of the default setting of $\mathcal{G}$, followed by a list of the arms of $*\mathbf{k}_{\mathcal{G}}$.

Under the heading 'INFORMATION FOR THE SPLITTING' follows a block containing information on the splitting of the star $*\mathbf{k}_{\mathcal{G}}$ into wave-vector stars $*\mathbf{k}_{\mathcal{H}}$ of the subgroup, *cf.* Equ. (7.6).

Next follow two blocks of the same type for the group and the subgroup (with the headings 'INFORMATION FOR THE SUPERGROUP' and 'INFORMATION FOR THE SUBGROUP'), containing information on the relevant little groups, the allowed little-group irreps, the chosen coset representatives of the decomposition of the group with respect to the little group and the full space-group irreps (optional).

The last block of the **Output**, entitled 'SUBDUCTION PROBLEM', contains the subduction coefficients and the corresponding subduction matrices for each irrep of the supergroup for the considered $*\mathbf{k}_{\mathcal{G}}$ vector.

Example The program `CORREL` is illustrated by the calculation of the subduction coefficients and matrices for the irrep $\boldsymbol{D}^{*\mathbf{X},1}$ of $P4bm$ ($\mathbf{k} = \mathbf{X}(0, 1/2, 0)$) in its subduction to the subgroup $P2$ of index 8.
The **Input** data includes:

1. The specification of the group-subgroup pair by the corresponding *IT*A numbers of the involved space groups and the transformation matrix ($\boldsymbol{P}, \boldsymbol{p}$) which relates the conventional bases of $\mathcal{G}$ and $\mathcal{H}$. The transformation matrices for a given group-subgroup pair and their index can be obtained from the program `SUBGROUPGRAPH` available on the Bilbao Crystallographic Server. There are seven subgroups $P2$ (No.3) of $P4bm$ (No.100) of index 8 distributed into 4 different classes of conjugate subgroups. Here, we consider the symmetry break

$P4bm > P2$ with

$$(\boldsymbol{P}, \boldsymbol{p}) \;=\; \left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \end{array}\right) .$$

2. The wave-vector **X** is specified by its primitive coefficients $(0, \frac{1}{2}, 0)$.

In the first block of the **Output** file the program lists the generators, general positions of $P4bm$ and $P2$ as (3x4) matrix-column pairs. The transformation matrix $(\boldsymbol{P}, \boldsymbol{p})$ is printed in the same form. The coefficients of its translation part are printed as multiples of $\frac{1}{24}$(*e.g.* $\frac{1}{2}$ is listed as 12). The two arms of ***X** are given by their conventional coefficients ***X**= $\{(0, \frac{1}{2}, 0), (\frac{1}{2}, 0, 0)\}$.
The splitting of the ***X** in the subgroup wave-vector stars ***S1** and ***S2**, Equ. (7.6), is indicated in the next block:

$$*\mathbf{X} = 1\_*\mathbf{S1} \oplus 1\_*\mathbf{S2} \ ,$$

where each $*\mathbf{k}_{\mathcal{H}}$ is preceded by its multiplicity in $*\mathbf{k}_{\mathcal{G}}$. In our case $(*\mathbf{X} \mid *\mathbf{S1}) = (*\mathbf{X} \mid *\mathbf{S2}) = 1$. The star $*\mathbf{S1} = (1, 0, 0)$ is equivalent to the $\mathbf{\Gamma}$ wave vector of $P2$. The star $*\mathbf{S2} = (0, 0, \frac{1}{2})$ is also a special one and corresponds to the point **Z** in CDML notation (*cf.* the Brillouin-zone database available on the Bilbao Crystallographic Server).

The next block includes the data on the little group and (optionally) the full-group irreps of $P4bm$ for the **X** wave vector. The little and full-group irreps of ***S1** and ***S2** of the subgroup $P2$, relevant for the subduction, are given in the block 'Information about the subgroup'. The presentation of the data follows the form and the sequence already discussed and illustrated in Section 7.2. There is one 4-dimensional full group irrep (***X**)(1) (*cf.* the example of the program REPRES). For each subgroup star ***S1** and ***S2** there exist two irreps labeled as (***Si**)(j), i,j=1,2, *i.e.* there are altogether 4 one-dimensional irreps of $P2$ which can take part in the decomposition of (***X**)(1) (*cf.* Equ. (7.4)). The irrep (***S1**)(1) corresponds to the identity irrep of $P2$.

The last block of the output file includes the subduction coefficients $(*\mathbf{k}_{\mathcal{G}},\, i \mid *\mathbf{k}_{\mathcal{H}},\, j)$ and the subduction matrices $\boldsymbol{S}$. The subduced irrep $(*\mathbf{X})(1) \downarrow P2$ splits into the four irreps of the subgroup, each appearing with multiplicity 1:

$$\begin{aligned} &(*\mathbf{X})(1) \downarrow P2 \\ &\quad \sim (*\mathbf{S1})(1) \oplus (*\mathbf{S1})(2) \oplus (*\mathbf{S2})(1) \oplus (*\mathbf{S2})(2) \ . \end{aligned} \tag{7.9}$$

The subduction matrix $\boldsymbol{S}$ is shown in two parts: a matrix with numerical values gives one possible (non-zero) solution for the subduction matrix. The irrep indices of its columns follow the order of the irreps in the direct-sum decomposition of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},\, i} \downarrow \mathcal{H}$ (Equ. (7.9)). The block-diagonal (unitary) matrix with complex parameters expressed by letters, is related to the uniqueness of $\boldsymbol{S}$. The freedom in the determination of the rectangular matrices $\boldsymbol{S}^{*\mathbf{k}_{\mathcal{H}},\, j}$ (7.8) is given by the corresponding sub-blocks. Their

dimensions equal the multiplicities of $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{H}},j}$ in $\boldsymbol{D}^{*\mathbf{k}_{\mathcal{G}},i}\downarrow\mathcal{H}$. In our example all irreps of the subgroup in Equ. (7.9) are of dimension 1 and the corresponding rectangular matrices are reduced to single columns. The freedom in their determination is given by single complex numbers (or phase factors if the normalization condition is imposed) as the multiplicities of the irreps $(*\mathbf{Si})(j)$ in $(*\mathbf{X})(1)$ equal 1.

7.4 Direct product of representations

7.4.1 The problem

There are a number of physical applications of the representation theory of space groups that are based on the analysis of the Kronecker product of space-group representations. A well-known example is related to the determination of selection rules for various physical processes in crystalline materials as infrared absorption, Raman scattering, neutron scattering, electron scattering, *etc* (see *e.g.* Birman and Berenson (1974), Cracknell (1974)). The essential step of the selection-rules derivations consists in the reduction of Kronecker products of space-group representations into irreducible constituents. Consider the irreps $\boldsymbol{D}^{*\mathbf{k},m}$ and $\boldsymbol{D}^{*\mathbf{k}',m'}$ of the space group $\mathcal{G}$ spanned by the sets of basis functions $\{\phi_1^{k_1,m},\ldots,\phi_{r_m}^{k_s,m}\}$ and $\{\phi_1^{k'_1,m'},\ldots,\phi_{r'_{m'}}^{k'_{s'},m'}\}$.[2] The set of all bilinears $\{\phi_1^{k_1,m}\phi_1^{k'_1,m'},\ldots,\phi_{r_m}^{k_s,m}\phi_{r'_{m'}}^{k'_{s'},m'}\}$ form a carrier space of the the so-called Kronecker (direct or tensor) product representation $\boldsymbol{D}^{*\mathbf{k},m}\otimes\boldsymbol{D}^{*\mathbf{k}',m'}$ of $\mathcal{G}$. It is in general a reducible representation with dim $(\boldsymbol{D}^{*\mathbf{k},m}\otimes\boldsymbol{D}^{*\mathbf{k}',m'})=(s\times r_m)(s'\times r'_{m'})$. In order to decompose the direct-product representation into irreducible constituents one first determines the so-called *reduction coefficients of the Clebsch-Gordon series* $(*\mathbf{k}m,*\mathbf{k}'m'|*\mathbf{k}''m'')$ (in the following referred to as *reduction coefficients* for short). The reduction coefficients are integers that indicate the irreps $\boldsymbol{D}^{*\mathbf{k}'',m''}$ that appear in the decomposition of the Kronecker product:

$$\begin{aligned}\boldsymbol{D}^{*\mathbf{k},m}\otimes\ \boldsymbol{D}^{*\mathbf{k}',m'}&\\ \sim\oplus_{*\mathbf{k}'',m''}[\boldsymbol{E}(*\mathbf{k}m,*\mathbf{k}'m'|*\mathbf{k}''m'')\otimes\ \boldsymbol{D}^{*\mathbf{k}'',m''}]\ .&\end{aligned}\tag{7.10}$$

In order to complete the decomposition, one further determines the *Clebsch-Gordan coefficients*. They define the correct linear combination of bilinear products $(\phi_\mu^{k_\sigma,m}\phi_{\mu'}^{k'_{\sigma'},m'})$ which transform according to the irreps $\boldsymbol{D}^{*\mathbf{k}'',m''}$. The Clebsch-Gordon coefficients can be suitably assembled into a matrix $\boldsymbol{C}$ that transforms the direct product (7.10) into a fully reduced form:

$$(\boldsymbol{D}^{*\mathbf{k},m}\otimes\boldsymbol{D}^{*\mathbf{k}',m'})\boldsymbol{C}=\boldsymbol{C}[\oplus\boldsymbol{E}(*\mathbf{k}m,*\mathbf{k}'m'|*\mathbf{k}''m'')\otimes\boldsymbol{D}^{*\mathbf{k}'',m''}].\tag{7.11}$$

Here the direct sum is over all stars $*\mathbf{k}''$, and over all allowable irreps $\boldsymbol{D}^{*\mathbf{k}'',m''}$ which may arise for a given $*\mathbf{k}''$. The identity matrix $\boldsymbol{E}(l)$ is of dimension l.

[2] Here $s(s')$ give the number of arms of $*\mathbf{k}(*\mathbf{k}')$, $r_m(r'_{m'})$ stand for the dimension of the little-group irreps $\boldsymbol{D}^{\mathbf{k},m}$ $(\boldsymbol{D}^{\mathbf{k}',m'})$. The products $(s\times r_m)$ and $(s'\times r'_{m'})$ equal the dimensions of the full-group irreps $d^{*\mathbf{k},m}=$ dim $(\boldsymbol{D}^{*\mathbf{k},m})$ and $d^{*\mathbf{k}',m'}=$ dim $(\boldsymbol{D}^{*\mathbf{k}',m'})$.

The theory of the decomposition of Kronecker products and the related reduction coefficients has been developed during the second half of the last century. Details on the different approaches and references to the numerous contributions to that field can be found *e.g.* in Bradley and Cracknell (1972) or CDML. The work involved in the construction of Kronecker products tables for space groups is rather tedious and requires a considerable expertise in some aspects of the representation theory of space groups. Probably this is the reason that the only systematic and relatively complete compilations of Kronecker product tables for the space groups are given in the Volumes 2, 3 and 4 of the Kronecker Product Tables (Davies and Cracknell (1979), Cracknell and Davies (1979) and Davies and Cracknell (1980)). The reductions of ordinary Kronecker products of the irreps of the special wave vectors in the representation domains of all 230 space groups are given in Volume 2 and 3 of the series. In Volume 4 the reductions of the symmetrized squares and cubes of the special wave vectors are listed. The tables are computer produced and the method for their calculation is based on the subgroup method. However, the Kronecker Product Tables have become a bibliographic collector's item. In addition, for certain applications the published data are not sufficient and/or it is necessary to have the data in an electronic form. The program `DIRPRO` carries out the reductions of ordinary Kronecker products of space-group irreps for any wave vector (in or outside of the representation domain). The program calculates the related wave-vector selection rules (see below) and the reduction coefficients. The program `DIRPRO` is designed to compute also the Clebsch-Gordon coefficients. For the moment this option is not included in the implemented version of `DIRPRO` on the Bilbao Crystallographic server.

7.4.2 The method

For the decomposition of the Kronecker product of two space-group irreps and the determination of the corresponding reduction coefficients we use a modification of the full-group method (*cf.* Birman (1974) for details and a mathematical background of the approach). The reduction procedure applied in `DIRPRO` is rather similar to the one used for the solution of the subduction problem (Section 7.3). The reason is obvious: in both cases it is necessary to decompose a reducible representation into irreducible constituents. The essential differences concern the construction of the reducible representation.
The determination of the reduction coefficients of an ordinary Kronecker product (7.10) of space-group irreps is carried out in two steps.

Wave-vector selection rules

The first step in the reduction procedure is the determination of the wave-vector stars $*\mathbf{k}''$ that occur in the splitting of the direct product $*\mathbf{k}\otimes *\mathbf{k}'$. One defines $^*\mathbf{k}$-*reduction coefficients* $(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')$ for the formal description of the splitting:

$$*\mathbf{k} \otimes *\mathbf{k}' = \sum_{*\mathbf{k}''} (*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')\ *\mathbf{k}''. \tag{7.12}$$

The fact that the $s_{\mathbf{k}}s'_{\mathbf{k}'}$ arms of the direct product $*\mathbf{k} \otimes *\mathbf{k}'$ must be expressible in terms of entire stars, results in the following relation for $(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')$:

$$s_{\mathbf{k}}s'_{\mathbf{k}'} = \sum_{*\mathbf{k}''}(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')\ s''_{\mathbf{k}''}. \tag{7.13}$$

The $*\mathbf{k}$-reduction coefficients are integers and are determined by direct inspection.

Reduction coefficients

The number N of unknown reduction coefficients equals the sum over the numbers of allowed irreps for each of the stars $*\mathbf{k}''$ that appear in the splitting of the Kronecker product. The method of linear equations is used for the determination of the reduction coefficients. The first q equations follow from the dimensionality conservation conditions for each of the resultant wave-vector stars $*\mathbf{k}''_i$, $i = 1, \ldots, q$:

$$\begin{aligned}\sum_{m''}(*\mathbf{k}m, *\mathbf{k}'m' \mid *\mathbf{k}''m'')d^{*\mathbf{k}'', m''} \\ = r_{\mathbf{k}m}r'_{\mathbf{k}'m'}(*\mathbf{k}*\mathbf{k}' \mid *\mathbf{k}'')s''_{\mathbf{k}''}.\end{aligned} \tag{7.14}$$

Here $d^{*\mathbf{k}'', m''}$ is the dimension of $\boldsymbol{D}^{*\mathbf{k}'', m''}$, and $r_{\mathbf{k}m}$ and $r'_{\mathbf{k}'m'}$ are the dimensions of the little group irreps of the factors $\boldsymbol{D}^{*\mathbf{k}, m}$ and $\boldsymbol{D}^{*\mathbf{k}', m'}$.
The rest of the equations for the reduction coefficients is obtained from the defining relation (7.10) rewritten for the characters of $\boldsymbol{D}^{*\mathbf{k}, m} \otimes \boldsymbol{D}^{*\mathbf{k}', m'}$ and the resultant irreps:

$$\begin{aligned}\chi^{(*\mathbf{k}, m)\otimes(*\mathbf{k}', m')}(g) = \sum(*\mathbf{k}m, *\mathbf{k}'m'|*\mathbf{k}''m'')\chi^{*\mathbf{k}'', m''}(g) \\ \text{where } \chi^{(*\mathbf{k}, m)\otimes(*\mathbf{k}', m')}(g) = \chi^{*\mathbf{k}, m}(g)\chi^{*\mathbf{k}', m'}\ (g),\ g \in \mathcal{G}.\end{aligned} \tag{7.15}$$

Trial and error methods are used for the selection of the necessary $(N-q)$ independent linear equations for the calculation of the reduction coefficients. The search is carried out among equations of the type (7.15) taken for different elements of $\mathcal{G}$. A Gauss elimination procedure is used for the solution of the system of linear equations for the reduction coefficients.

7.4.3 The program DIRPRO

The **Input** data of DIRPRO includes the specification of the space group $\mathcal{G}$ by its *IT*A number and the data for the wave vectors. The $\mathbf{k}$-vector coefficients could be referred to the primitive bases of reciprocal space (as found in CDML), to the centered dual basis (conventional $\mathbf{k}$-vector coefficients). As an option the program displays the full-group representations (not just the representations of the little groups) for the generators of the space group. There is also an option to consider the symmetrized Kronecker squares if $*\mathbf{k} = *\mathbf{k}'$.

The structure of the **Output** of DIRPRO follows that of CORREL. The first block lists the information about the space group $\mathcal{G}$ including its space-group number and lattice type, generators and translational coset representatives $(\boldsymbol{W}, \boldsymbol{w})$ given in (3x4) matrix form. The **k**-vectors are specified by their input coefficients and those referred to the dual basis of the default setting of $\mathcal{G}$. The arms of the wave-vector stars $*\mathbf{k}$ and $*\mathbf{k}'$ are also shown. The wave-vector selection rules are displayed in the block with the heading 'INFORMATION FOR THE SPLITTING'. Each of the resulting $*\mathbf{k}''$ stars is specified by its **k**-vector coefficients referred to the dual basis of $\mathcal{G}$. Next follows the block containing information on the representations of the space group $\mathcal{G}$ for $*\mathbf{k}$, $*\mathbf{k}'$ and all $*\mathbf{k}''$ stars that appear in the splitting of the direct product. The data consists of the corresponding little groups, the allowed little-group irreps, the chosen coset representatives of the decomposition of the group with respect to the little group and the full space-group irreps given for the generators (optional). The last block of the **Output**, named 'REDUCTION PROBLEM', shows the decompositions of all possible direct products $\boldsymbol{D}^{*\mathbf{k},m} \otimes \boldsymbol{D}^{*\mathbf{k}',m'}$ (for each allowed m and m') into direct sums of irreducible constituents.

7.5 Illustrative examples

The databases and computer packages on space- and point-group representations, form the set of basic modules which is used further in different programs on the Bilbao Crystallographic Server for applications of representation theory to specific problems of solid-state physics and chemistry. For example, symmetry-mode analysis of atomic displacements of crystalline solids could be very helpful for the proper interpretation of infrared and Raman experimental results. The program SAM computes the symmetry-adapted modes at the Γ point and studies their infrared and Raman activity. The program NEUTRON (Kirov *et al.*, 2003) computes the phonon selection rules applicable in inelastic neutron-scattering experiments. The software packages SYMMODES (Capillas *et al.*, 2003) and AMPLIMODES (Orobengoa *et al.*, 2009) performs a group-theoretical and symmetry-mode analysis of structural phase transitions. In the following, we illustrate the usefulness of the group-subgroup computer tools available on the Bilbao Crystallographic Server (the program SUBGROUPGRAPH, for more details see *e.g.* Aroyo *et al.* (2006a)) and the correlation relations obtained by CORREL in treating phase-transition problems.

Consider a continuous or quasi-continuous phase transition between two crystalline phases whose symmetry groups are group-subgroup related $\mathcal{G} > \mathcal{H}$. The order parameter which drives the transition (*i.e.* it is related to the symmetry-breaking distortion with respect to the high symmetry phase) is known as the *primary order parameter* and it is associated with an irrep $\boldsymbol{D}^{*\mathbf{k},m}$ of $\mathcal{G}$, the so-called *active* irrep. The direction of the order parameter below the transition determines the space-group symmetry $\mathcal{H}$ which is also known as the *isotropy subgroup* of the order parameter. A subgroup $\mathcal{H}$ is an isotropy subgroup of $\boldsymbol{D}^{*\mathbf{k},m}$ of $\mathcal{G}$ if and only if: (i) the subduction multiplicity of the identity irrep of $\mathcal{H}$ in $\boldsymbol{D}^{*\mathbf{k},m} \downarrow \mathcal{H}$ is non-zero, and (ii) there exists no supergroup $\mathcal{Z}$ of $\mathcal{H}$ in the group-subgroup graph of maximal subgroups of $\mathcal{G} > \mathcal{H}$ with the same subduction multiplicity of the identity irrep of $\mathcal{Z}$ in $\boldsymbol{D}^{*\mathbf{k},m} \downarrow \mathcal{Z}$. These conditions are

known as subduction and chain-subduction criteria (see *e.g.* Birman, 1978). In the analysis of the symmetry break $\mathcal{G} \longrightarrow \mathcal{H}$ one should consider all possible distortions compatible with the symmetry $\mathcal{H}$. Some distortions are related to order parameters associated with irreps different from that of the primary order parameter and are known as *secondary order parameters*. Their isotropy subgroups are in general supergroups of the space group of the low-symmetry phase in the group-subgroup graph $\mathcal{G} > \mathcal{H}$. The symmetry analysis of the primary and secondary order parameters of a transformation between a high- and a low-symmetry phase of given space-group symmetries, is known as the inverse Landau problem (Ascher and Kobayashi, 1977). The following two 'classical' examples demonstrate how the results of the programs `SUBGROUPGRAPH` and `CORREL`, can be applied for the solution of the inverse Landau problem.

Example 1 The crystal structure of $BaTiO_3$ is of perovskite type. Above 120 ℃, $BaTiO_3$ has the ideal paraelectric cubic phase ($Pm\bar{3}m$, No.221). As temperature is lowered, $BaTiO_3$ assumes tetragonal, then orthorhombic and finally trigonal structures with slightly deformed unit cells. The three structures are ferroelectric with different directions of the spontaneous polarization axes. The possible transformation matrices for the symmetry break $Pm\bar{3}m > P4mm$ (No.99) of index 6 are listed by the program `SUBGROUPGRAPH`. The three different $P4mm$ subgroups of $Pm\bar{3}m$ corresponding to the three domain orientations of the tetragonal phase are conjugated in $Pm\bar{3}m$. Here, we consider the case of the identity transformation matrix between the conventional bases of $Pm\bar{3}m$ and $P4mm$. The low-symmetry space group $P4mm$ is a *translationengleiche* subgroup (or *t*-subgroup for short) of $Pm\bar{3}m$ but it is not a maximal subgroup: the chain of maximal subgroups is of the form: $Pm\bar{3}m > P4/mmm > P4mm$. The correlation relations calculated by `CORREL` for $Pm\bar{3}m > P4mm$ with **k**-vector $\mathbf{\Gamma}$=(0,0,0) indicate the candidates for the irreps of $Pm\bar{3}m$ associated to the possible primary and secondary order parameters. The subduction multiplicity of the identity irrep of $P4mm$ is equal to 1 for three different irreps of $Pm\bar{3}m$: (***GM**)(1) (which is the identity irrep), (***GM**)(6) and (***GM**)(9) (here we use the irrep notation of `CORREL`). The application of the chain-subduction criteria distinguishes between primary and secondary order parameters. The obvious isotropy group of (***GM**)(1) is the high-symmetry group itself and the irrep (***GM**)(1) is related to the possible volume change that would occur during the transformation. The run of `CORREL` for the pair $Pm\bar{3}m > P4/mmm$ shows that the group $P4/mmm$ is the isotropy sugroup for (***GM**)(6), and the associated secondary order parameter corresponds to the onset of tetragonal strain during the transformation. Finally, the physical distortion characterized by (***GM**)(9) can be related to the onset of non-zero polarization and be associated to the primary-order parameter. The columns of the subduction matrices of the irreps (***GM**)(1), (***GM**)(6) and (***GM**)(9) corresponding to the identity irrep of the isotropy groups indicate the directions of the order parameters in the irrep carrier spaces. One should note that the specific form of the order-parameter direction depends on the choice of the irrep matrices.

The application of the subduction and chain-subduction conditions for the symmetry break $Pm\bar{3}m > R3m$, index 8, shows that the primary distortions related to the onset

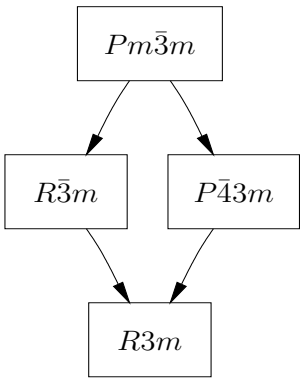


Figure 7.4: Graph of maximal subgroups for the group-subgroup pair $Pm\bar{3}m > R3m$, index 8.

of polarization along one of the main-diagonal directions of the cube is associated also to (***GM**)(9) but with order parameter direction (a,a,a). There are three more irreps of $Pm\bar{3}m$ whose subduction multiplicities of the identity irrep of $R3m$ are different from zero: (***GM**)(1), (***GM**)(4) and (***GM**)(8). Their isotropy groups $Pm\bar{3}m$, $P\bar{4}3m$ and $R\bar{3}m$ are determined from the results of `CORREL` for the pairs $Pm\bar{3}m > P\bar{4}3m$ and $Pm\bar{3}m > R\bar{3}m$. The graph $Pm\bar{3}m > R3m$ derived by the program `SUBGROUPGRAPH` (Fig.7.5), shows that the isotropy subgroups $P\bar{4}3m$ and $R\bar{3}m$ are intermediate supergroups of $R3m$ which indicates that the corresponding order parameters are secondary ones.

Example 2 As a second example we consider another well-studied, both experimentally and theoretically, phase transition, namely that of $SrTiO_3$. In that case the transformation is associated with the **k**-vector point **R**=($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) which is at the border of the Brillouin zone. The high-symmetry space group is $Pm\bar{3}m$ and the low-symmetry phase is tetragonal, of space-group symmetry $I4/mcm$ (No. 140) with a doubling of the unit cell, *i.e.* $I4/mcm$ is a general-type subgroup of $Pm\bar{3}m$ of index 6. The analysis of the group-subgroup relations by `SUBGROUPGRAPH` shows that there are 4 different classes of conjugate $I4/mcm$ subgroups. Each class consists of three different subgroups, related to the three possible doublings of the unit cell of the subgroup. The different classes are distinguished by the different origin choices of the subgroup with respect to the group. For the specific transformation we are considering, $I4/mcm$ has the lattice vectors (**a**-**b**, **a**+**b**, 2**c**) with an origin shift ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) with respect to the $Pm\bar{3}m$ basis. `SUBGROUPGRAPH` lists the following chain of maximal subgroups: $Pm\bar{3}m > P4/mmm > I4/mcm$. The correlation relations derived by `CORREL` for the ***R**-irreps shows that only the 3-dimensional irrep (***R**)(7) of $Pm\bar{3}m$ subduces the identity irrep of $I4/mcm$, with an order parameter direction (a,0,0). Obviously, this is the irrep associated with the primary order parameter, as the only intermediate supergroup $P4/mmm$ of $I4/mcm$ is a *t*-subgroup of $Pm\bar{3}m$. The possible secondary order parameters with $P4/mmm$ as isotropy subgroup, could be associated only with Brillouin-zone centre irreps of $Pm\bar{3}m$. The results of `CORREL` for **Γ**=(0,0,0) for the pairs $Pm\bar{3}m > I4/mcm$ and $Pm\bar{3}m > P4/mmm$ (tetragonal lattice vectors (**a**-**b**, **a**+**b**, **c**), with no origin shift) show that the possible secondary order parameters are associated with (***GM**)(1) (volume change) and (***GM**)(6) (tetragonal distortion).

References

Altmann, S. L. & Herzig, P. (1994). Point-Group Theory Tables. Oxford: Clarendon Press.

Aroyo, M. I., Perez-Mato, J. M., Capillas, C., Kroumova, E., Ivantchev, S., Madariaga, G., Kirov, A. and Wondratschek, H. (2006a). *Z. Kristallogr.* **221**, 15-27.

Aroyo, M. I., G., Kirov, A., Capillas, C., Perez-Mato, J.M. and Wondratschek, H. (2006b). *Acta Cryst.* A**62**, 115-128.

Aroyo, M. I. & Wondratschek, H. (1995). Crystallographic viewpoints in the classification of space–group representations. *Z. Kristallogr.* **210**, 243–254.

Ascher, E. and Kobayashi, J. (1977). *J.Phys. C: Solid State Physics* **10**, 1349-1363.

Birman, J. L. (1974). *Theory of Crystal Space Groups and Infrared and Raman Lattice Processes of Insulating Crystals* in *Handbuch der Physik*, Bd.XXV/2b. Edited by S. Flüge. Berlin: Springer Verlag.

Birman, J. L. (1978) *Group Theory in the Landau Thermodynamic Theory of Continuous Phase Transitions in Crystals*, in *Group-theoretical Methods in Physics*, eds. P. Kramers and A. Reickers. Berlin: Springer Verlag, 203-222.

Birman, J. L. and Berenson, R. (1974). *Phys. Rev.* **B9** 4512-4517.

Bouckaert, L. P., Smoluchowski, R. & Wigner, E. P. (1936). Theory of Brillouin zones and symmetry properties of wave functions in crystals. *Phys. Rev.* **50**, 58–67.

BC, Abbreviation of: Bradley, C. J. & Cracknell, A. P. (1972). The *Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups.* Oxford: Clarendon Press.

Buerger, M. J. (1956). *Elementary Crystallography.* New York: J. Wiley & Sons.

Burckhardt, J. J. (1966). *Die Bewegungsgruppen der Kristallographie.* Basel: Birkhäuser Verlag.

Capillas, C., Kroumova E., Perez-Mato J. M., Aroyo, M. I., Stokes, H. S. and Hatch, D. (2003). *J. Appl. Cryst.* **36**, 953-954.

Cracknell, A. P. (1974) *Advan. Phys.* **23** 673-866.

Cracknell, A. P. and Davies, B. L. (1979). *Kronecker Product Tables.* Volume 3. *General Wave Vector Selection Rules and Reductions of Kronecker Products for Irreducible Representations of Triclinic, Monoclinic, Tetragonal, Trigonal and Hexagonal Space Groups.* New York: IFI/Plenum.

CDML, abbreviation of: 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.

Davies, B. L., Cracknell, A. P. (1979). *Kronecker Product Tables.* Volume 2. *General Wave Vector Selection Rules and Reductions of Kronecker Products for Irreducible Representations of Orthorhombic and Cubic Space Groups.* New York: IFI/Plenum.

Davies, B. L. and Cracknell, A. P. (1980). *Kronecker Product Tables.* Volume 4. *General Symmetrized Powers of Irreducible Representations of Space Groups.* New York: IFI/Plenum.

IT A, abbreviation of: *International Tables for Crystallography.* Vol. A, *Space–Group Symmetry* (2002). Ed. Th. Hahn. 5th ed. Dordrecht: Kluwer Academic Publishers.

International Tables of Crystallography, Vol. A1 (2004). *Symmetry relations between space groups.* Edited by H. Wondratschek and U. Müller. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography, Vol. E (2002). *Subperiodic Groups.* Edited by V. Kopsky and D. Litvin. Dordrecht: Kluwer Academic Publishers.

Kim, S. K. (1999). *Group-Theoretical Methods and Applications to Molecules and Crystals.* Cambridge: University Press.

Kirov, A., Aroyo, M. I. and Perez-Mato, J. M. (2003). *J. Appl. Cryst.* **36** 1085-1089.

Koster, G. F., Dimmock, J. O., Wheeler, R. G. and Statz, H. (1963). *Properties of the Thirty-two Point Groups.* Cambridge: M.I.T. Press.

Kovalev, O. V. (1986). *Irreducible and Induced Representations and Corepresentations of Fedorov Groups.* Moscow: Nauka (in Russian).

Lomont, J. S. (1959). *Applications of Finite Groups.* New York: Academic Press.

Mulliken, R. S. (1933). *Phys. Rev.* **43** 279-302.

Orobengoa, D., Capillas, C., Aroyo M. I. and Perez-Mato, J. M. (2009) AMPLIMODES: symmetry-mode analysis on the Bilbao Crystallographic Server. *J. Appl. Cryst.*, A**42**, 820-833.

Raghavacharyulu, I. V. V. (1961). Representations of space groups. *Can. J. Phys.* **39**, 830–840.

Rigault, G. (1980). *Metric Tensor and Symmetry Operations in Crystallography.* Pamphlet No. 10, publ. for IUCr. Cardiff: University College Cardiff Press.

Stokes, H. T. & Hatch, D. M. (1988). *Isotropy Subgroups of the 230 Crystallographic Space Groups.* Singapore: World Scientific.

Streitwolf, H.-W. (1967). *Gruppentheorie in der Festkörperphysik.* Leipzig: Akademische Verlagsges.

Wintgen, G. (1941). Zur Darstellungstheorie der Raumgruppen. *Math. Annalen* **118**, 195–215.

Zak, J. (1960). Method to obtain the character tables of nonsymmorphic space groups. *J. math. Phys.* **1**, 165–171.

Zak, J., Casher, A., Glück, M. & Gur, Y. (1969). *The Irreducible Representations of Space Groups.* New York: Benjamin.

Index