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Teaching Edition

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Edited by

MOIS I. AROYO

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Preface

This Teaching Edition (hereafter referred to as the TE) is the successor to the *Brief Teaching Edition of Volume A* (which was last revised in 2005), although new material, substantial revisions and reorganisation of the text has resulted in a book that is quite different in structure and content to its predecessor. It focuses on the particular topic of symmetry, owing to its fundamental role in crystallography, and provides a unified and coherent introduction to the symmetry information found in three volumes of *International Tables for Crystallography*: the basic crystallographic data for the plane and space groups in Volume A (*IT* A), the symmetry relations between space groups treated in Volume A1 (*IT* A1) and the subperiodic-group data found in Volume E (*IT* E). It also introduces the Symmetry Database, which forms part of the online version of *International Tables for Crystallography* at https://it.iucr.org.

This Teaching Edition is designed for graduate (and postgraduate) students, and young researchers who have some awareness of the basics of symmetry and diffraction and who need to use crystallographic symmetry methods in their work. The TE can thus serve as an interface between elementary crystallography textbooks and the texts in *IT* A, A1 and E. Sufficient up-to-date and accessible references to further specialized sources are provided for those who need to go deeper into the subject, and to textbooks and basic crystallographic literature that could be helpful for those who need a course in basic crystallography or introduction to the mathematics that is required. The fruitful combination of tables for practical use and a didactic introduction to symmetry makes this TE a handy tool with which researchers and students can familiarize themselves with the use of crystallographic symmetry and its practical applications.

Part 1 of the TE is based on the material of the introductory part of the sixth edition of *IT* A, with additional explanations and illustrative examples to provide the reader with practical experience in the use of crystallographic symmetry data. The fundamental concepts of group theory, focusing on those properties that are of particular importance for crystallography, are introduced in the first chapter. The matrix formalism, which provides efficient instruments for the analytical description of crystallographic symmetry, is the subject of Chapter 1.2. Chapter 1.3 offers an introduction to the structure of space groups and their various classification schemes, focusing on the classifications into space-group types, geometric crystal classes and Bravais types of lattices. Chapter 1.4 deals with various crystallographic terms and the symbols used to present the symmetry data in the space-group tables of *IT* A. The purpose of Chapter 1.5 is to provide the mathematical tools needed to work out how crystallographic data are transformed if the coordinate system is changed. Chapter 1.6 offers a detailed presentation of methods for determining the symmetry of single-domain crystals from diffraction data. The tables of general reflection conditions shown in this chapter also include ‘diffraction symbols’ (previously known as ‘extinction symbols’), and four examples of space-group determination from real intensity data are analysed. Chapter 1.7 deals with applications of crystallographic symmetry, including symmetry relations between space groups, as treated in *IT* A1, and subperiodic groups, as covered in *IT* E. Possible applications of the subperiodic groups in the description of crystal systems with rod and layer symmetry are discussed. Finally, magnetic groups, including magnetic subperiodic groups and magnetic space groups, are briefly introduced.

The material of Part 2 focuses on the presentation of the tables of crystallographic symmetry data found in Volumes A, A1 and E, including descriptions of the symbols and terms found in the tables and guides for their use. Representative sets of tables of varying complexity are included that will be useful for teaching about crystallographic symmetry. The guide to the space-group tables of Volume A is very similar to that given in Chapter 2.1 of *IT* A and is complemented by the tables for 7 of the plane groups and 35 of the space groups. In Chapter 2.2, the data for the maximal subgroups and minimal supergroups in *IT* A1 are described and illustrated using the examples of $P3_112$ (151) and $P3_121$ (152). The guide to the arrangement of the data specifying relations between Wyckoff positions in *IT* A1 uses the tables of $P6_3/mmc$ (194) and $Cmcm$ (63) as examples. The subperiodic-group tables in *IT* E are described in Chapter 2.3 and are illustrated by the tables of the rod group $\not{p}mc2_1$ (No. 17), and of the layer groups $p2_1/b11$ (No. 17) and $pbam$ (No. 44). Finally, Chapter 2.4 gives a brief description of the Symmetry Database, which provides online access to data for the crystallographic space and point groups that extend and enhance the symmetry information given in the printed editions of *IT* A and A1.

It is a great pleasure to express my gratitude to all authors of the TE; their contributions were indispensable for the successful completion of this project. We should dedicate this book to the memory of those authors who, to my deep regret, are not among us anymore: H. Wondratschek (KIT, Karlsruhe), Th. Hahn (RWTH, Aachen), A. Looijenga-Vos (Rijksuniversiteit Groningen), V. Kopský (Academy of Science, Prague) and H. Flack (University of Geneva).

My thanks should be extended to the International Union of Crystallography and its Editorial Office for making this Teaching Edition possible, and in particular to C. P. Brock (University of Kentucky, Lexington), P. R. Strickland and N. J. Ashcroft (IUCr Editorial Office, Chester) for providing much of the initial stimulus for this work, and for their confidence and support during it. I am particularly grateful to Nicola Ashcroft for the careful and dedicated technical editing of this book, and for her help and professionalism.

Helpful discussions were held with and invaluable comments were received from B. Souvignier (Radboud University, Nijmegen), M. Nespolo (Université de Lorraine, Nancy), U. Shmueli (Tel Aviv University), M. Glazer (Oxford University) and many others, for which I thank them most sincerely. The constant encouragement and understanding during my work on this Teaching Edition from colleagues and friends at the Universidad del País Vasco are also gratefully acknowledged. The preparation of this book was supported by projects funded by the Universidad del País Vasco, the Government of the Basque Country and the Spanish Ministry of Science and Innovation.

MOIS I. AROYO
Editor, *Teaching Edition of International Tables for Crystallography*

1.1. A general introduction to groups

Bernd Souvignier

In this chapter we give a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, we discuss those properties of groups that are of particular interest in crystallography. To readers interested in a more elaborate treatment of the theoretical background, the standard textbooks by Armstrong (2010), Hill (1999) or Sternberg (2008) are recommended; an account from the perspective of crystallography can also be found in Müller (2013).

1.1.1. Introduction

Crystal structures may be investigated and classified according to their symmetry properties. But in a strict sense, crystal structures in nature are never perfectly symmetric, due to impurities, structural imperfections and especially their finite extent. Therefore, symmetry considerations deal with *idealized* crystal structures that are free from impurities and structural imperfections and that extend infinitely in all directions. In the mathematical model of such an idealized crystal structure, the atoms are replaced by points in a three-dimensional point space and this model will be called a *crystal pattern*.

A symmetry operation of a crystal pattern is a transformation of three-dimensional space that preserves distances and angles and that leaves the crystal pattern as a whole unchanged. The symmetry of a crystal pattern is then understood as the collection of all symmetry operations of the pattern.

The following simple statements about the symmetry operations of a crystal pattern are almost self-evident:

(*a*) If two symmetry operations are applied successively, the crystal pattern is still invariant, thus the combination of the two operations (called their *composition*) is again a symmetry operation.

(*b*) Every symmetry operation can be reversed by simply moving every point back to its original position.

These observations (together with the fact that leaving all points in their position is also a symmetry operation) show that the symmetry operations of a crystal pattern form an algebraic structure called a *group*.

1.1.2. Basic properties of groups

Although groups occur in innumerable contexts, their basic properties are very simple and are captured by the following definition.

Definition. Let $\mathcal{G}$ be a set of elements on which a binary operation is defined which assigns to each pair (g, h) of elements the composition $g \circ h \in \mathcal{G}$. Then $\mathcal{G}$, together with the binary operation $\circ$, is called a *group* if the following hold:

(i) the binary operation is associative, *i.e.* $(g \circ h) \circ k = g \circ (h \circ k)$;

(ii) there exists a *unit element* or *identity element* $e \in \mathcal{G}$ such that $g \circ e = g$ and $e \circ g = g$ for all $g \in \mathcal{G}$;

(iii) every $g \in \mathcal{G}$ has an inverse element, denoted by g^{-1}, for which $g \circ g^{-1} = g^{-1} \circ g = e$.

In most cases, the composition of group elements is regarded as a *product* and is written as $g \cdot h$ or even gh instead of $g \circ h$. An exception is groups where the composition is addition, *e.g.* a group of translations. In such a case, the composition $\mathbf{a} \circ \mathbf{b}$ is more conveniently written as $\mathbf{a} + \mathbf{b}$.

Examples

(i) The set $\mathbb{Z}$ of all integers forms a group with addition as operation. The identity element is 0, the inverse element for $a \in \mathbb{Z}$ is $-a$.

(ii) The group $3m$ of all symmetries of an equilateral triangle is a group with the composition of symmetry operations as binary operation. The group contains six elements, namely three reflections, two rotations and the identity element. It is schematically displayed in Fig. 1.1.2.2.

(iii) The set of all real $n \times n$ matrices with determinant $\neq 0$ is a group with matrix multiplication as operation. This group is called the *general linear group* and denoted by $\mathrm{GL}_n(\mathbb{R})$.

If a group $\mathcal{G}$ contains finitely many elements, it is called a *finite group* and the number of its elements is called the *order* of the group, denoted by $|\mathcal{G}|$. A group with infinitely many elements is called an *infinite group*.

For a group element g, its *order* is the smallest integer $n > 0$ such that $g^n = e$ is the identity element. If there is no such integer, then g is said to be of *infinite order*.

The group operation is not required to be *commutative*, *i.e.* in general one will have $gh \neq hg$. However, a group $\mathcal{G}$ in which $gh = hg$ for all g, h is said to be a *commutative* or *abelian group*.

The inverse of the product gh of two group elements is the product of the inverses of the two elements in reversed order, *i.e.* $(gh)^{-1} = h^{-1}g^{-1}$.

Groups of small order may be displayed by their *multiplication table*, which is a square table with rows and columns indexed by the group elements and where the intersection of the row labelled by g and of the column labelled by h is the product gh. It follows immediately from the invertibility of the group elements that each row and column of the multiplication table contains every group element precisely once.

Examples

(i) The group of rotations leaving an equilateral triangle invariant consists of the rotations by 0, 120 and 240°, which are denoted by 1, 3^+ and 3^-, respectively. Its multiplication table is

	1	3^+	3^-
1	1	3^+	3^-
3^+	3^+	3^-	1
3^-	3^-	1	3^+

Note that in this and all subsequent examples of crystallographic point groups we will use *Seitz symbols* (*cf.* Section 1.4.2.2) for the symmetry operations and

1.2. Crystallographic symmetry

Hans Wondratschek and Mois I. Aroyo

1.2.1. Crystallographic symmetry operations

Geometric mappings have the property that for each point X of the space, and thus of the object, there is a uniquely determined point $\tilde{X}$, the *image point*. If also for each image point $\tilde{X}$ there is a uniquely determined preimage or original point X, then the mapping is called *reversible*. Examples of non-reversible mappings are *projections*, *cf.* Section 1.4.5.

A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In Volume A of *International Tables for Crystallography* (2016), abbreviated as *IT* A, and in this edition, the term 'isometry' is used.

Isometries are a special kind of affine mappings. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but distances along the same line are preserved.

A mapping is called a *symmetry operation* of an object if (i) it is an isometry, and (ii) it maps the object onto itself. Instead of 'maps the object onto itself' one frequently says 'leaves the object invariant (as a whole)'.

Real crystals are finite objects in physical space, which because of the presence of impurities and structural imperfections such as disorder, dislocations *etc.* are not perfectly symmetric. In order to describe their symmetry properties, real crystals are modelled as blocks of ideal, infinitely extended periodic structures, known as *ideal crystals* or (ideal) crystal structures. Crystal patterns are models of crystal structures in point space. In other words, while the crystal structure is an infinite periodic spatial arrangement of the atoms (ions, molecules) of which the real crystal is composed, the crystal pattern is the related model of the ideal crystal (crystal structure) consisting of a strictly three-dimensional periodic set of points in point space. If the growth of the ideal crystal is undisturbed, then it forms an *ideal macroscopic crystal* and displays its ideal shape with planar faces.

Both the symmetry operations of an ideal crystal and of a crystal pattern are called *crystallographic symmetry operations*. The symmetry operations of the ideal macroscopic crystal form the finite point group of the crystal, those of the crystal pattern form the (infinite) space group of the crystal pattern. Because of its periodicity, a crystal pattern always has translations among its symmetry operations.

The symmetry operations are divided into two main kinds depending whether they preserve or not the so-called *handedness* or *chirality* of chiral objects. *Isometries of the first kind* or *proper isometries* are those that preserve the handedness of chiral objects: *e.g.* if a right (left) glove is mapped by one of these isometries, then the image is also a right (left) glove of equal size and shape. Isometries that change the handedness, *i.e.* the image of a right glove is a left one, of a left glove is a right one, are called *isometries of the second kind* or *improper isometries*. Improper isometries cannot be performed in space physically but can nevertheless be observed as symmetries of objects.

The notion of *fixed points* is essential for the characterization of symmetry operations. A point X is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{X}$ is the same as the original point X: $\tilde{X} = X$. The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

Crystallographic symmetry operations are also characterized by their *order*: a symmetry operation W is of *order* k if its application k times results in the identity mapping, *i.e* $\mathsf{W}^k = \mathsf{I}$, where I is the identity operation, and $k > 0$ is the smallest number for which this equation is fulfilled.

There are eight different types of isometries that may be crystallographic symmetry operations:

(1) The *identity operation* I maps each point of the space onto itself, *i.e.* the set of fixed points is the whole space. It is the only operation whose order is 1. The identity operation is a symmetry operation of the first kind. It is a symmetry operation of any object and although trivial, it is indispensable for the group properties of the set of symmetry operations of the object (*cf.* Section 1.1.2).

(2) A *translation* t is characterized by its translation vector $\mathbf{t}$. Under translation every point of space is shifted by $\mathbf{t}$, hence a translation has no fixed point. A translation is a symmetry operation of infinite order as there is no number $k \neq 0$ such that $t^k = \mathsf{I}$ with translation vector $\mathbf{o}$. It preserves the handedness of any chiral object.

(3) A *rotation* is an isometry which leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle ϕ. Because of the periodicity of crystals, the rotation angles of crystallographic rotations are restricted to $\phi = k \times 2\pi/N$, where N = 2, 3, 4 or 6 and k is an integer which is relative prime to N (for details, see Section 1.3.3.1). A rotation of rotation angle $\phi = k \times 2\pi/N$ is of order N and is called an N-fold rotation. A rotation preserves the handedness of any chiral object.

The rotations are also characterized by their *sense of rotation*. The adopted convention for *positive* (*negative*) sense of rotation follows the mathematical convention for *positive* (*negative*) sense of rotation: the sense of rotation is positive (negative) if the rotation is counter-clockwise (clockwise) when viewed down the rotation axis.

(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is called the *screw axis*. The translation vector is called the *screw vector* or the *intrinsic translation component* $\mathbf{w}_g$ (of the screw rotation), *cf.* Section 1.2.2.3. A screw rotation has no fixed points because of its translation component. However, the screw axis is invariant pointwise under the so-called *reduced symmetry operation* of the screw rotation: it is the rotation obtained from the screw rotation by removing its intrinsic translation component.

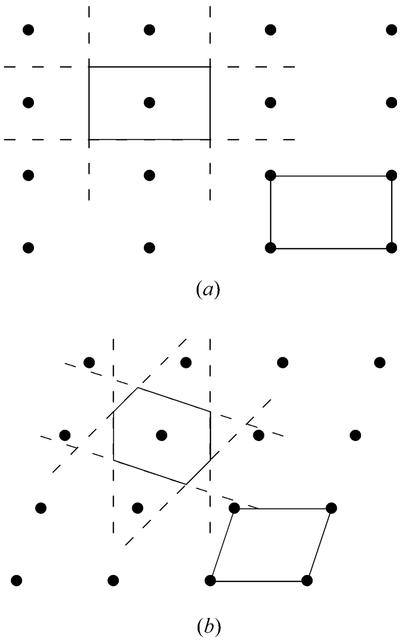


Figure 1.3.2.2
Voronoï domains and primitive unit cells for a rectangular lattice (*a*) and an oblique lattice (*b*).

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}.$$

1.3.2.3. Unit cells

A lattice $\mathbf{L}$ can be used to subdivide $\mathbb{V}^3$ into cells of finite volume which all have the same shape. The idea is to define a suitable subset $\mathbf{C}$ of $\mathbb{V}^3$ such that the translates of $\mathbf{C}$ by the vectors in $\mathbf{L}$ cover $\mathbb{V}^3$ without overlapping. Such a subset $\mathbf{C}$ is called a *unit cell* of $\mathbf{L}$, or, in the more mathematically inclined literature, a *fundamental domain* of $\mathbb{V}^3$ with respect to $\mathbf{L}$. Two standard constructions for such unit cells are the *primitive unit cell* and the *Voronoï domain* (which is also known by many other names).

Definition

Let $\mathbf{L}$ be a lattice in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(i) The set $\mathbf{C} := \{x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \mid 0 \le x, y, z < 1\}$ is called the *primitive unit cell* of $\mathbf{L}$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The primitive unit cell is the parallelepiped spanned by the vectors of the given basis.

(ii) The set $\mathbf{C} := \{\mathbf{w} \in \mathbb{V}^3 \mid |\mathbf{w}| \le |\mathbf{w} - \mathbf{v}| \text{ for all } \mathbf{v} \in \mathbf{L}\}$ is called the *Voronoï domain* or *Dirichlet domain* or *Wigner–Seitz cell* or *Wirkungsbereich* or *first Brillouin zone* (for the case of reciprocal lattices in dual space, see Section 1.3.2.5) of $\mathbf{L}$ (around the origin).

The Voronoï domain consists of those points of $\mathbb{V}^3$ that are closer to the origin than to any other lattice point of $\mathbf{L}$.

See Fig. 1.3.2.2 for examples of these two types of unit cells in two-dimensional space.

It should be noted that the attribute 'primitive' for a unit cell is often omitted. The term 'unit cell' then either denotes a primitive unit cell in the sense of the definition above or a slight generalization of this, namely a cell spanned by vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ which are not necessarily a lattice basis. This will be discussed in detail in the next section.

The construction of the Voronoï domain is independent of the basis of $\mathbf{L}$, as the Voronoï domain is bounded by planes bisecting the line segment between the origin and a lattice point and perpendicular to this segment. The boundaries of the Voronoï domain and its translates overlap, thus in order to get a proper fundamental domain, part of the boundary has to be excluded from the Voronoï domain.

The volume V of the unit cell can be expressed both *via* the metric tensor and *via* the cell parameters. One has

$$\begin{aligned} V^2 &= \det \boldsymbol{G} \\ &= a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma) \end{aligned}$$

and thus

$$V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}.$$

Although the cell parameters depend on the chosen lattice basis, the volume of the unit cell is not affected by a transition to a different lattice basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. As remarked in Section 1.3.2.1, two lattice bases are related by an integral basis transformation $\boldsymbol{P}$ of determinant ±1 and therefore $\det \boldsymbol{G}' = \det(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P}) = \det \boldsymbol{G}$, *i.e.* the determinant of the metric tensor is the same for all lattice bases.

Assuming that the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a *right-handed* system, the volume can also be obtained *via*

$$V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}).$$

1.3.2.4. Primitive and centred lattices

The definition of a lattice as given in Section 1.3.2.1 states that a lattice consists precisely of the integral linear combinations of the vectors in a lattice basis. However, in crystallographic applications it has turned out to be convenient to work with bases that have particularly nice metric properties. For example, many calculations are simplified if the basis vectors are perpendicular to each other, *i.e.* if the metric tensor has all non-diagonal entries equal to zero. Moreover, it is preferable that the basis vectors reflect the symmetry properties of the lattice. By a case-by-case analysis of the different types of lattices a set of rules for convenient bases has been identified and bases conforming with these rules are called *conventional bases*. The conventional bases are chosen such that in all cases the integral linear combinations of the basis vectors are lattice vectors, but it is admitted that not all lattice vectors are obtained as integral linear combinations.

To emphasize that a basis has the property that the vectors of a lattice are precisely the integral linear combinations of the basis vectors, such a basis is called a *primitive basis* for this lattice.

If the conventional basis of a lattice is not a primitive basis for this lattice, the price to be paid for the transition to the conventional basis is that in addition to the integral linear combinations of the basis vectors one requires one or more *centring vectors* in order to obtain all lattice vectors. These centring vectors have non-integral (but rational) coordinates with respect to the conventional basis. The name *centring* vectors reflects the fact that the additional vectors are usually the centres of the unit cell or of faces of the unit cell spanned by the conventional basis.

Definition

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be linearly independent vectors in $\mathbb{V}^3$.

(i) A lattice $\mathbf{L}$ is called a *primitive lattice* with respect to a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ if $\mathbf{L}$ consists precisely of all integral linear combinations of $\mathbf{a}, \mathbf{b}, \mathbf{c}$, *i.e.* if $\mathbf{L} = \mathbf{L}_P = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$.

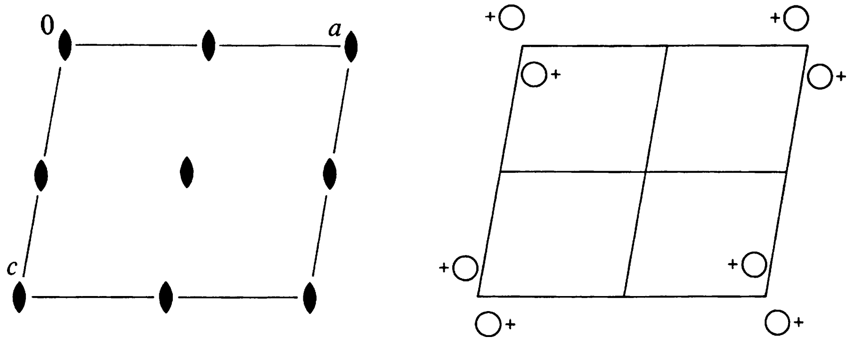


Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group *P*2, No. 3 (unique axis *b*, cell choice 1).

position orbits are *non-characteristic*, *i.e.* their eigensymmetry groups are supergroups of the space groups. (An introduction to terms like eigensymmetry groups, characteristic and non-characteristic orbits, and further discussion of space groups with non-characteristic general-position orbits are given in Section 1.4.4.4 of *IT* A.)

(2) The graphical presentation of the general-position points of cubic groups is more difficult: three different parameters are required to specify the height of the points along the projection direction. To make the presentation clearer, the general-position points are grouped around points of higher site symmetry and represented in the form of polyhedra. For the general-position diagrams of *IT* A for most of the space groups the initial general point is taken as 0.048, 0.12, 0.089, and the polyhedra are centred at 0, 0, 0 (and its equivalent points). Additional general-position diagrams are shown for space groups with special sites different from 0, 0, 0 that have site-symmetry groups of equal or higher order. Consider, for example, the two general-position diagrams of the space group $I4_132$ (214) shown in Fig. 1.4.2.8. The polyhedra of the left-hand diagram are centred at special points of highest site-symmetry, namely, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points in the unit cell. The site-symmetry groups are of the type 32 leading to polyhedra in the form of *twisted trigonal antiprisms* (*cf.* Table 3.2.3.2 of *IT* A). The polyhedra (sphenoids) of the right-hand diagram are attached to the origin 0, 0, 0 and its equivalent points in the unit cell, site-symmetry group of the type 3. The fractions attached to the polyhedra indicate the heights of the high-symmetry points along the projection direction (*cf.* Section 2.1.3.6 for further explanations of the diagrams).

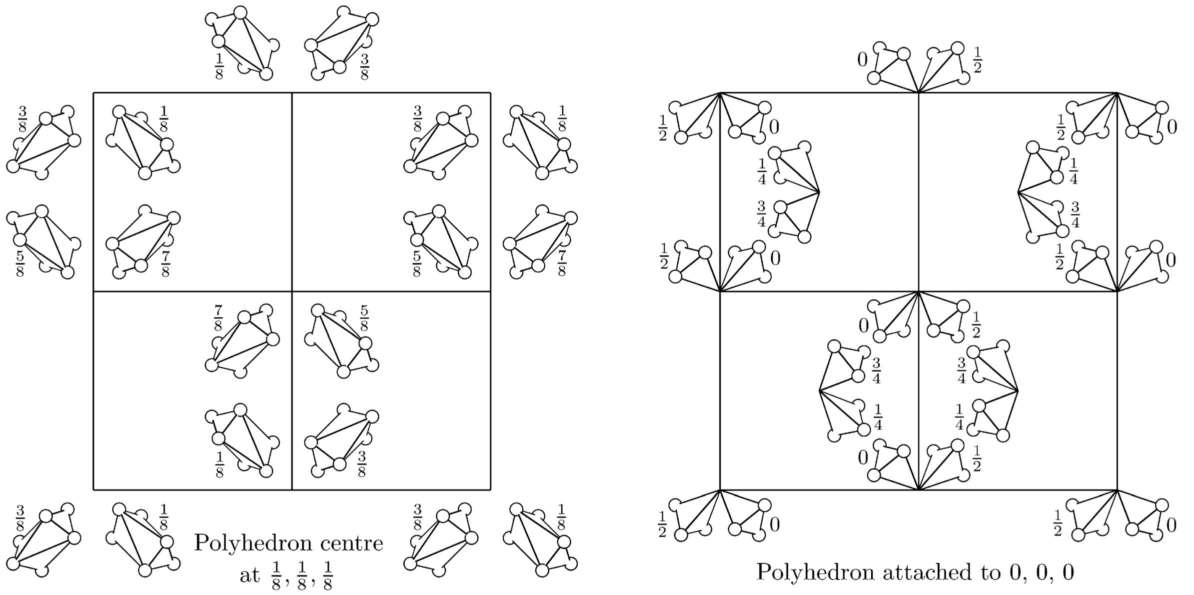
1.4.3. Generation of space groups

By Hans Wondratschek

In group theory, a *set of generators* of a group is a set of group elements such that each group element may be obtained as a finite ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of h generators g_j ($j = 1, 2, \ldots, h$). Thus,

$$W = g_h^{k_h} \cdot g_{h-1}^{k_{h-1}} \cdot \ldots \cdot g_p^{k_p} \cdot \ldots \cdot g_3^{k_3} \cdot g_2^{k_2} \cdot g_1,$$

where the powers k_j are positive or negative integers (including zero). The description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point group $m\bar{3}m$ can be described by two generators. Different choices of generators are possible. For the



Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

Polyhedron attached to 0, 0, 0

Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (site-symmetry group .3.).

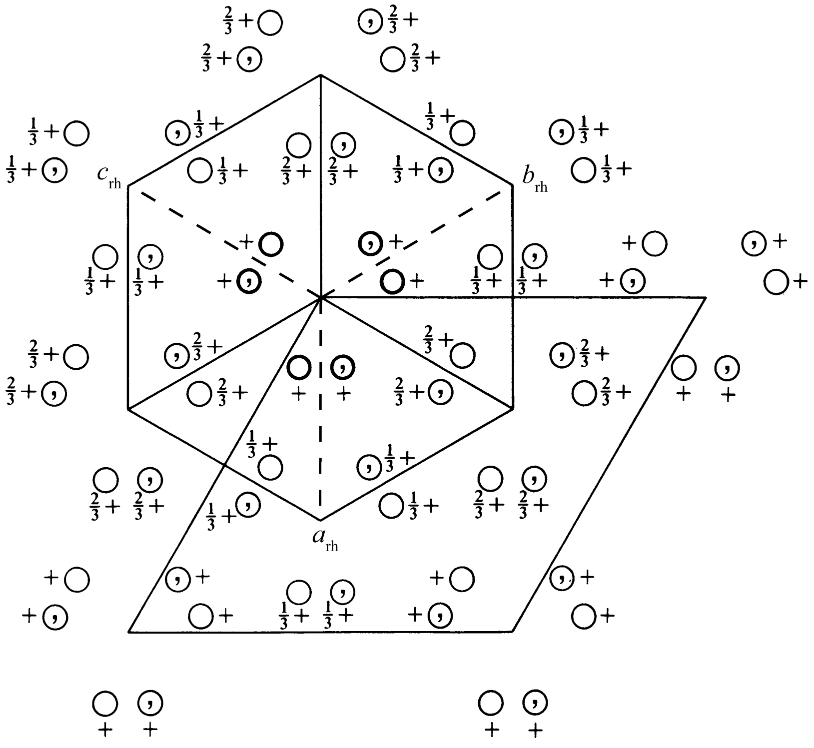


Figure 1.5.3.3

General-position diagram of the space group $R3m$ (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting: $\mathbf{a}_{\rm rh} = \frac{1}{3}(2\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{b}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{c}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} - 2\mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$.

gonal cell ($|\mathbf{a}_{\rm hex}| = |\mathbf{b}_{\rm hex}|$; $\mathbf{c}_{\rm hex} \perp \mathbf{a}_{\rm hex}$, $\mathbf{b}_{\rm hex}$; $\gamma = 120^\circ$) with a volume three times larger than that of the primitive rhombohedral cell. The second presentation is given with a primitive rhombohedral cell with $a_{\rm rh} = b_{\rm rh} = c_{\rm rh}$ and $\alpha_{\rm rh} = \beta_{\rm rh} = \gamma_{\rm rh}$. The relation between the two types of cell is illustrated in Fig. 1.5.3.3 for the space group $R3m$ (160). In the hexagonal cell, the coordinates of the special position with site symmetry $3m$ are 0, 0, z, whereas in the rhombohedral cell the same special position has coordinates x, x, x. If we refer to the transformations of the primitive rhombohedral cell cited in Table 1.5.1.1, we observe two different centrings with three possible orientations R_1, R_2 and R_3 which are related by ±120° to each other. The two kinds of centrings, called *obverse* and *reverse*, are illustrated in Fig. 1.5.1.6. A rotation of 180° around the threefold axis relates the obverse and reverse descriptions of the rhombohedral lattice. The obverse triple R cells have lattice points at 0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$, whereas the reverse R cells have lattice points at 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$. The triple hexagonal cell R_1 of the obverse setting (*i.e.* $\mathbf{a}_{\rm hex} = \mathbf{a}_{\rm rh} - \mathbf{b}_{\rm rh}$, $\mathbf{b}_{\rm hex} = \mathbf{b}_{\rm rh} - \mathbf{c}_{\rm rh}$, $\mathbf{c}_{\rm hex} = \mathbf{a}_{\rm rh} + \mathbf{b}_{\rm rh} + \mathbf{b}_{\rm rh}$) has been used in the description of the rhombohedral space groups in *IT* A (*cf.* Table 1.5.1.1 and Fig. 1.5.3.3).

1.5.3.2. Examples

Example 1: Transformations between different settings of $P2_1/c$

In the space-group tables of Part 2 (see also the space-group tables of *IT* A), the monoclinic space group $P2_1/c$ (14) is described in six different settings: for each of the 'unique axis b' and 'unique axis c' settings there are three descriptions specified by different cell choices (*cf.* Section 1.5.4 and Table 1.5.4.1; for more details see Section 2.1.3.15 of *IT* A). The different settings are identified by the appropriate full Hermann–Mauguin symbols. The basis transformations $(\boldsymbol{P}, \boldsymbol{p})$ between the different settings are completely specified by the linear part of the transformation, the 3 × 3 matrix $\boldsymbol{P}$ [*cf.* equation (1.5.1.4)], as all settings of $P2_1/c$ refer to the same origin, *i.e.* $\boldsymbol{p} = \boldsymbol{o}$. The transformation matrices $\boldsymbol{P}$ necessary for switching between the different descriptions of $P2_1/c$ can either be read off directly or constructed from the transformation-matrix data listed in Table 1.5.1.1.

The transformation from $P12_1/c1$ (unique axis b, cell choice 1) to $P112_1/a$ (unique axis c, cell choice 1) is illustrated by the following example. The change of the direction of the screw axis 2_1 indicates that the unique direction $\mathbf{b}$ transforms to the unique direction $\mathbf{c}$, while the glide vector along $\mathbf{c}$ transforms to a glide vector along $\mathbf{a}$. These changes are reflected in the transformation matrix $\boldsymbol{P}$ between the basis $\mathbf{a}_b$, $\mathbf{b}_b$, $\mathbf{c}_b$ of $P12_1/c1$ and $\mathbf{a}_c$, $\mathbf{b}_c$, $\mathbf{c}_c$ of $P112_1/a$, which can be obtained directly from Table 1.5.1.1:

$$(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c) = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\boldsymbol{P} = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$
$$= (\mathbf{c}_b, \mathbf{a}_b, \mathbf{b}_b).$$

The matrix for the inverse transformation is

$$\boldsymbol{Q} = \boldsymbol{P}^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

(i) *Transformation of point coordinates.* From $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$, *cf.* equation (1.5.1.5), it follows that

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix} = \begin{pmatrix} z_b \\ x_b \\ y_b \end{pmatrix}.$$

For example, the representative coordinate triplets of the special Wyckoff position $2d$ $\bar{1}$ of $P12_1/c1$ transform exactly to the representative coordinate triplets of the special

1.6. Introduction to the theory and practice of space-group determination

Uri Shmueli, Howard D. Flack and John C. H. Spence

1.6.1. Overview

This chapter describes and discusses several methods of symmetry determination of single-domain crystals. A detailed presentation of symmetry determination from diffraction data is followed by a brief discussion of intensity statistics, ideal as well as non-ideal, with an application of the latter to real intensity data from a $P\bar{1}$ crystal structure. Several methods of retrieving symmetry information from a solved crystal structure are then discussed. This is followed by a discussion of chemical and physical restrictions on space-group symmetry, including some aids in symmetry determination, and by a brief section on pitfalls in space-group determination.

The following two sections deal with reflection conditions. The first presents briefly the theoretical background of conditions for possible general reflections and their corresponding derivation. A relevant example follows. The second presents some examples of tabulations of general reflection conditions and possible space groups.

These are followed by a concise section on space-group determination in macromolecular crystallography.

Next, a description and illustration of symmetry determination based on electron-diffraction methods are presented. These are principally focused on convergent-beam electron diffraction.

The chapter concludes with four examples of space-group determination from real intensity data, employing methods described in the previous sections of this chapter.

This chapter deals only with single crystals. A supplement (Flack, 2015) deals with twinned crystals and those displaying a specialized metric.

1.6.2. Symmetry determination from single-crystal studies

By Uri Shmueli and Howard D. Flack

1.6.2.1. Symmetry information from the diffraction pattern

The extraction of symmetry information from the diffraction pattern takes place in three stages.

In the first stage, the unit-cell dimensions are determined and analysed in order to establish to which Bravais lattice the crystal belongs. The Bravais lattice symbol consists of two characters. The first is the first letter of the name of a crystal family and the second is the centring mode of a conventional unit cell. For example, the Bravais-lattice types *tP* and *tI* belong to the tetragonal family and have conventional unit-cell parameters $a = b$, c, $\alpha = \beta = \gamma = 90^\circ$.

Knowledge of the Bravais lattice leads to a conventional choice of the unit cell, primitive or centred. The determination of the Bravais lattice of the crystal is achieved by the process of cell reduction, in which the lattice is first described by a primitive unit cell, and then linear combinations of the unit-cell vectors are taken to reduce the metric tensor (and the cell dimensions) to a standard form. From the relationships amongst the elements of the metric tensor, one obtains the Bravais lattice, together with a conventional choice of the unit cell, with the aid of standard tables [*e.g.* those in *International Tables for Crystallography* Volume A (2016), hereafter abbreviated as *IT* A]. A detailed description of cell reduction is given in Chapter 3.1 of *IT* A and in Part 9 of earlier editions (*e.g.* Burzlaff *et al.*, 2002). Formally, cell reduction leads to a conventional lattice basis for the crystal, primitive or centred, depending on its Bravais-lattice type. An alternative approach (Le Page, 1982) seeks the Bravais lattice directly from the cell dimensions by searching for all the twofold axes present. All these operations are automated in software. Regardless of the technique employed, at the end of the process one obtains an indication of the Bravais lattice and a unit cell in a conventional setting for the crystal system. These are usually good indications which, however, must be confirmed by an examination of the distribution of diffracted intensities as outlined below.

In the second stage, it is the point-group symmetry of the intensities of the Bragg reflections which is determined. We recall that the average reduced intensity of a pair of Friedel opposites (*hkl* and $\overline{hkl}$) is given by

$$\begin{aligned}|F_{\rm av}(\mathbf{h})|^2 &= \tfrac{1}{2}[|F(\mathbf{h})|^2 + |F(\bar{\mathbf{h}})|^2]\\ &= \sum_{i,j}[(f_i + f_i')(f_j + f_j') + f_i''f_j'']\cos[2\pi\mathbf{h}(\boldsymbol{r}_i - \boldsymbol{r}_j)] \equiv A(\mathbf{h}),\end{aligned} \tag{1.6.2.1}$$

where the atomic scattering factor of atom *j*, taking into account resonant scattering (sometimes called anomalous scattering or, in old literature, anomalous dispersion), is given by

$$\mathbf{f}_j = f_j + f_j' + if_j'',$$

the wavelength-dependent components f_j' and f_j'' being the real and imaginary parts, respectively, of the contribution of atom *j* to the resonant scattering, $\mathbf{h}$ contains in the (row) matrix (1×3) the diffraction orders (*hkl*) and $\boldsymbol{r}_j$ contains in the (column) matrix (3×1) the coordinates (x_j, y_j, z_j) of atom *j*. The components of the $\mathbf{f}_j$ are assumed to contain implicitly the displacement parameters. Equation (1.6.2.1) can be found *e.g.* in Okaya & Pepinsky (1955), Rossmann & Arnold (2001) and Flack & Shmueli (2007). It follows from (1.6.2.1) that

$$|F_{\rm av}(\mathbf{h})|^2 = |F_{\rm av}(\bar{\mathbf{h}})|^2 \text{ or } A(\mathbf{h}) = A(\bar{\mathbf{h}}),$$

regardless of the contribution of resonant scattering. Hence the averaging introduces a centre of symmetry in the (averaged) diffraction pattern. We must thus mention the well known Friedel's law, which states that $|F(\mathbf{h})|^2 = |F(\bar{\mathbf{h}})|^2$ and which is only a reasonable approximation for noncentrosymmetric crystals if resonant scattering is negligibly small. This law holds well for centrosymmetric crystals, independently of the resonant-scattering contribution. In fact, working with the average of Friedel opposites, one may determine the Laue group of the diffraction pattern by comparing the intensities of reflections which should be symmetry equivalent under each of the Laue groups. These are the 11 centrosymmetric point groups: $\bar{1}$, $2/m$, mmm, $4/m$, $4/mmm$, $\bar{3}$, $\bar{3}m$, $6/m$, $6/mmm$, $m\bar{3}$ and $m\bar{3}m$. For example, the reflections of which the intensities are to be

1.7. Applications of crystallographic symmetry: space-group symmetry relations, subperiodic groups and magnetic symmetry

HANS WONDRATSCHEK, ULRICH MÜLLER, DANIEL B. LITVIN, VOJTECH KOPSKÝ AND CAROLYN PRATT BROCK

1.7.1. Subgroups and supergroups of space groups

BY HANS WONDRATSCHEK

Relations between crystal structures play an important role for the comparison and classification of crystal structures, the analysis of phase transitions in the solid state, the understanding of topotactic reactions, and other applications. The relations can often be expressed by group–subgroup relations between the corresponding space groups. Such relations may be recognized from relations between the lattices and between the point groups[1] of the crystal structures.

In the first five editions of Volume A of *International Tables for Crystallography*, subgroups and those supergroups of space groups that are space groups were listed for every space group. However, the listing was incomplete and it lacked additional information, such as, for example, possible unit-cell transformations and/or origin shifts involved. It became apparent that complete lists and more detailed data were necessary. Therefore, a supplementary volume of *International Tables for Crystallography* to Volume A was published: Volume A1, *Symmetry Relations between Space Groups* (2004; second edition 2010; abbreviated as *IT* A1). The listing of the subgroups and supergroups was thus discontinued in the sixth edition of Volume A (2016) (abbreviated as *IT* A).

Volume A1 consists of three parts. Part 1 covers the theory of space groups and their subgroups, space-group relations between crystal structures and the corresponding Wyckoff positions, and the Bilbao Crystallographic Server (http://www.cryst.ehu.es/). This server is freely accessible and offers access to computer programs that display the subgroups and supergroups of the space groups and other relevant data. Part 2 of Volume A1 contains complete lists of the maximal subgroups of the plane groups and space groups, including unit-cell transformations and origin shifts, if applicable. An overview of the group–subgroup relations is also displayed in diagrams. Part 3 contains tables of relations between the Wyckoff positions of group–subgroup-related space groups and a guide to their use. Chapter 2.2 of this Teaching Edition includes a guide to and several illustrative examples of the symmetry-relations tables of Volume A1.

Example

The crystal structures of silicon, Si, and sphalerite, ZnS, belong to space-group types $Fd\bar{3}m$ (O_h^7; No. 227) and $F\bar{4}3m$ (T_d^2; No. 216) with lattice parameters $a_{\rm Si}$ = 5.43 Å and $a_{\rm ZnS}$ = 5.41 Å. The structure of sphalerite (zinc blende) is obtained from that of silicon by replacing alternately half of the Si atoms by Zn and half by S, and by adjusting the lattice parameter (for details of the procedure, see Fig. 1.7.2.1, where the crystal-structure relation between diamond and zinc blende is illustrated). The strong connection between the two crystal structures is reflected in the relation between their space groups: the point group (crystal class) and the space group of sphalerite is a subgroup (of index 2) of that of silicon (ignoring the small difference in lattice parameters).

Data on subgroups and supergroups of the space groups are useful for the discussion of structural relations and phase transitions. It must be kept in mind, however, that group–subgroup relations only constitute symmetry relations. It is important, therefore, to ascertain that the consequential relations between the lattice parameters and between the atomic coordinates of the particles of the crystal structures also hold before a structural relation can be deduced from a symmetry relation.

Examples

NaCl and CaF_2 belong to the same space-group type, $Fm\bar{3}m$ (O_h^5; No. 225), and have lattice parameters $a_{\rm NaCl}$ = 5.64 Å and $a_{{\rm CaF}_2}$ = 5.46 Å. The ions, however, occupy unrelated positions and so the symmetry relation does not express a structural relation.

Pyrite, FeS_2, and solid carbon dioxide, CO_2, belong to the same space-group type, $Pa\bar{3}$ (T_h^6; No. 205). They have lattice parameters $a_{{\rm FeS}_2}$ = 5.42 Å and $a_{{\rm CO}_2}$ = 5.55 Å, and the particles occupy analogous Wyckoff positions. Nevertheless, the structures of these compounds are not related, because the positional parameters x = 0.386 of S in FeS_2 and x = 0.118 of O in CO_2 differ so much that the coordinations of the corresponding atoms are dissimilar.

To formulate group–subgroup relations some definitions are necessary. Subgroups and their distribution into conjugacy classes, normal subgroups, supergroups, maximal subgroups, minimal supergroups, proper subgroups, proper supergroups and index are defined for groups in general in Chapter 1.1. These definitions are used also for crystallographic groups like space groups. In the present section, the subgroup data of *IT* A1 are explained through many examples in order to enable the reader to use these data.

Examples

Maximal subgroups $\mathcal{H}$ of a space group $P1$ with basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are, among others, subgroups $P1$ for which $\mathbf{a}'' = p\mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, p prime. If p is not a prime number but a product of two integers $p = q \times r$, the subgroup $\mathcal{H}$ is not maximal because a proper subgroup $\mathcal{Z}$ of index q exists such that $\mathbf{a}' = q\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$. $\mathcal{Z}$ again has $\mathcal{H}$ as a proper subgroup of index r with $\mathcal{G} > \mathcal{Z} > \mathcal{H}$.

$P12_1/c1$ has maximal subgroups $P12_11$, $P1c1$ and $P\bar{1}$ with the same unit cell, whereas $P1$ is not a maximal subgroup of $P12_1/c1$: $P12_1/c1 > P12_11 > P1$; $P12_1/c1 > P1c1 > P1$; $P12_1/c1 > P\bar{1} > P1$. These are all possible chains of maximal subgroups for $P12_1/c1$ if the original translations are retained

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[1] The point group determines both the symmetry of the physical properties of the macroscopic crystal and the symmetry of its ideal shape. Each space group belongs to a point group.

In practice, small differences in the lattice parameters of $\mathcal{G}$ and $\mathcal{R}$ will occur, because lattice deviations can accompany a structural relationship.

1.7.2. Relations between Wyckoff positions for group–subgroup-related space groups

By Ulrich Müller

1.7.2.1. Symmetry relations between crystal structures

The crystal structures of two compounds are *isotypic* if their atoms are arranged in the same way and if they have the same or the enantiomorphic space group. The absolute values of the lattice parameters and interatomic distances may differ and small deviations are permitted for non-fixed coordinates of corresponding atoms. The axial ratios and interaxial angles must be similar. Two structures are *homeotypic* if the conditions for isotypism are relaxed because (Lima-de-Faria *et al.*, 1990): (1) their space groups differ, allowing for a group–subgroup relation; (2) the geometric conditions differ (axial ratios, interaxial angles, atomic coordinates); or (3) an atomic position in one structure is occupied in an ordered way by various atomic species in the other structure (substitution derivatives or after a misorder–order phase transition).[2]

Group–subgroup relations between the space groups of homeotypic crystal structures are particularly suited to disclosing the relationship. A standardized procedure to set forth such relations was developed by Bärnighausen (1980). The concept is to start from a simple, highly symmetrical crystal structure and to derive more complicated structures by distortions and/or substitutions of atoms. A tree of group–subgroup relations between the space groups involved, now called a *Bärnighausen tree*, serves as the main guideline. The highly symmetrical starting structure is called the *aristotype* after Megaw (1973) or *basic structure* after Buerger (1947, 1951) or, in the literature on phase transitions in physics, *prototype* or *parent structure*. The derived structures are the *hettotypes* or *derivative structures* or, in phase-transition physics, *distorted structures* or *daughter phases*. In Megaw's terminology, the structures mentioned in the tree form a *family of structures*.

Detailed instructions on how to form a Bärnighausen tree, the information that can be drawn from it and some possible pitfalls are given in Chapter 1.6 of the second edition of *IT* A1 (2010) and in the book by Müller (2013). In any case, setting up group–subgroup relations requires a thorough monitoring of how the Wyckoff positions develop from a group to a subgroup for every position occupied. The following examples give a concise impression of such relations.

1.7.2.2. Substitution derivatives

As an example, Fig. 1.7.2.1 shows the simple relation between diamond and zinc blende. This is an example of a substitution derivative. The reduction of the space-group symmetry from diamond to zinc blende is depicted by an arrow which points from the higher-symmetry space group of diamond to the lower-symmetry space group of zinc blende. The subgroup is *translationengleiche* of index 2, marked by *t*2 in the middle of the arrow. *Translationengleiche* means that the subgroup has the same translational lattice (the same size and dimensions of the primitive unit cell) but its crystal class is of reduced symmetry. The index [*i*] is the factor by which the total number of symmetry operations has been reduced, *i.e.* the subgroup has 1/*i* as many symmetry operations; as mentioned in Section 1.7.1, this is to be understood in the same way as 'the number of even numbers is half as many as the number of all integer numbers'.

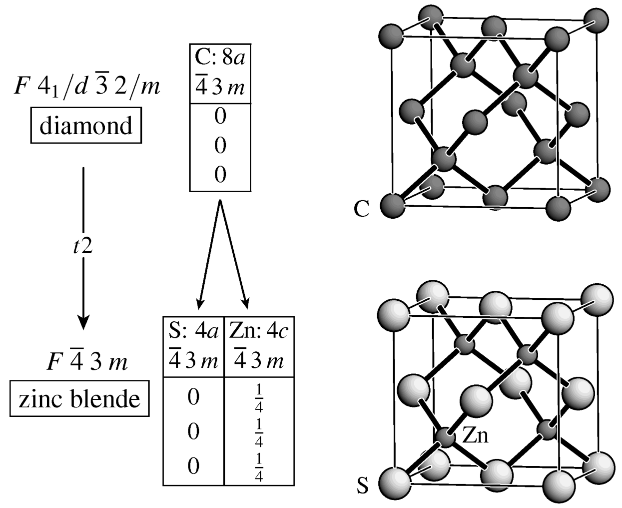

Figure 1.7.2.1
Group–subgroup relation from the aristotype diamond to its hettotype zinc blende. The numerical values in the boxes are atomic coordinates.

The consequences of the symmetry reduction on the positions occupied by the atoms are important. As shown in the boxes next to the space-group symbols in Fig. 1.7.2.1, the carbon atoms in diamond occupy the Wyckoff position 8*a* of the space group $F\,4_1/d\,\bar{3}\,2/m$. Upon transition to zinc blende, this position splits into two independent Wyckoff positions, 4*a* and 4*c*, of the subgroup $F\,\bar{4}\,3\,m$, rendering possible occupation by atoms of the two different species zinc and sulfur. The site symmetry $\bar{4}3m$ remains unchanged for all atoms.

Further substitutions of atoms require additional symmetry reductions. For example, in chalcopyrite, $CuFeS_2$, the zinc atoms of zinc blende have been substituted by copper and iron atoms. This implies a symmetry reduction from $F\bar{4}3m$ to its subgroup $I\bar{4}2d$; this requires one *translationengleiche* and two steps of *klassengleiche* group–subgroup relations, including a doubling of the unit cell.

1.7.2.3. Phase transitions

Fig. 1.7.2.2 shows derivatives of the cubic ReO_3 structure type that result from distortions of this high-symmetry structure. WO_3 itself does not adopt this structure, only several distorted variants. The first step of symmetry reduction involves a tetragonal distortion of the cubic ReO_3 structure resulting in the space group $P4/mmm$; no example with this symmetry is yet known. The second step leads to a *klassengleiche* subgroup of index 2 (marked *k*2 in the arrow), resulting in the structure of high-temperature WO_3, which is the most symmetrical known modification of WO_3. *Klassengleiche* means that the subgroup belongs

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[2] In the strict sense, two isotypic compounds do not have the same space group if their translation lattices (lattice parameters) differ. However, such a strict treatment would render it impossible to apply group-theoretical methods in crystal chemistry and crystal physics. Therefore, we treat isotypic and homeotypic structures as if their translation lattices were the same or related by an integral enlargement factor. For more details see the second edition of *IT* A1 (2010), Sections 1.2.7 and 1.6.4.1. We prefer the term 'misorder' instead of the usual 'disorder' because there still is order in the 'disordered' structure, although it is a reduced order.

2 and 4, or into three with multiplicity of 2 *etc.* If the unit cell of the subgroup is enlarged or reduced by a factor *f*, then the sum of the multiplicities must also be multiplied or divided by this factor *f*.

Part 3 of *IT* A1, *Relations between the Wyckoff positions*, contains tables for all space groups. For every one of them, all maximal subgroups are listed, including the corresponding coordinate transformations. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given. This includes the infinitely many maximal isomorphic subgroups, for which general formulae are given. Isomorphic subgroups are a special kind of *klassengleiche* subgroup that belong to the same or the enantiomorphic space-group type, *i.e.* group and subgroup have the same or the enantiomorphic space-group symbol; the unit cell of the subgroup is increased by some integral factor, which is p, p^2 or p^3 (p = prime number) in the case of maximal isomorphic subgroups.

1.7.3. Subperiodic groups

1.7.3.1. Relationships between space groups and subperiodic groups

By Daniel B. Litvin and Vojtech Kopský

IT A, *Space-Group Symmetry*, treats one-, two- and three-dimensional space groups. *IT* E, *Subperiodic Groups* (2010), treats two- and three-dimensional subperiodic groups: frieze groups (groups in two-dimensional space with translations in a one-dimensional subspace), rod groups (groups in three-dimensional space with translations in a one-dimensional subspace) and layer groups (groups in three-dimensional space with translations in a two-dimensional subspace). In the same way in which three-dimensional space groups are used to classify the atomic structure of three-dimensional crystals, the subperiodic groups are used to classify the atomic structure of other crystalline structures, such as liquid crystals, domain interfaces, twins and thin films. A brief description of the content and arrangement of the subperiodic-group tables of *IT* E, and several illustrative examples are given in Chapter 2.3.

In *IT* A, the relationship between the space group of a crystal and the point-group symmetry of individual points in the crystal is given by site symmetries, the point-group subgroups of the space group that leave the points invariant. In *IT* E, an analogous relationship is given between the space group of a crystal and the subperiodic-group symmetry of planes that transect the crystal. *IT* E contains *scanning tables* (with supplementary tables in Kopský & Litvin, 2004) from which the layer-group subgroups of the space group (called *sectional layer groups*) that leave the transecting planes invariant can be determined. The first attempts to derive sectional layer groups were made by Wondratschek (1971) and by using software written by Guigas (1971). Davies & Dirl (1993*a*,*b*) developed software for finding subgroups of space groups which was modified to find sectional layer groups. The use and determination of sectional layer groups have also been discussed by Janovec *et al.* (1988), Kopský & Litvin (1989) and Fuksa *et al.* (1993).

In Fig. 1.7.3.1, part of the scanning table for the space group $P\bar{3}m1$ (164) is given. From this one can determine the layer-group subgroups of $P\bar{3}m1$ that are symmetries of planes of orientation ($hkil$) = (0001). Vectors $\mathbf{a}'$ and $\mathbf{b}'$ are basic vectors of the translational subgroup of the layer-group symmetry of planes of this orientation. The vector $\mathbf{d}$ defines the *scanning direction* and is used to define the position of the plane within the crystal. The *linear orbit* is the set of all parallel planes obtained by applying all elements of the space group to any one plane. The *sectional layer group* is the layer subgroup of the space group that leaves the plane invariant.

Orientation orbit ($hkil$)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$	
(0001)	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$P\bar{3}m1$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{3}m1$	L72
					$[s\mathbf{d}, -s\mathbf{d}]$	$p3m1$	L69

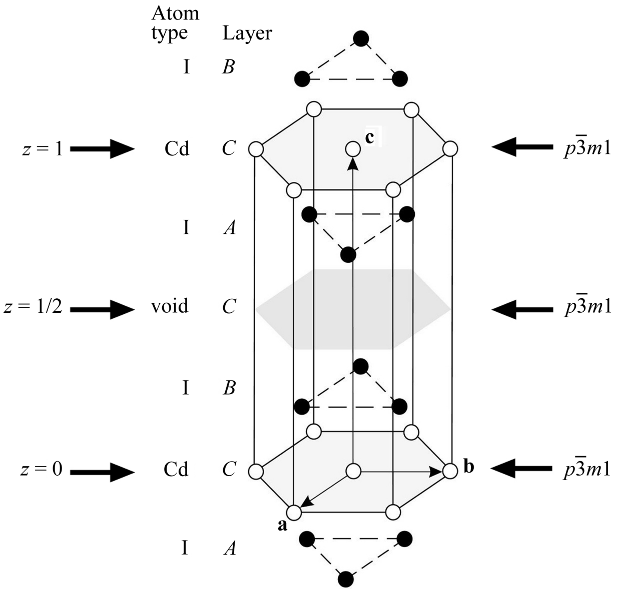

Figure 1.7.3.1
The scanning table for the space-group type $P\bar{3}m1$ (164) and orientation orbit (0001), and the structure of cadmium iodide, CdI_2. Cadmium and iodine ions are denoted by open and filled circles, respectively.

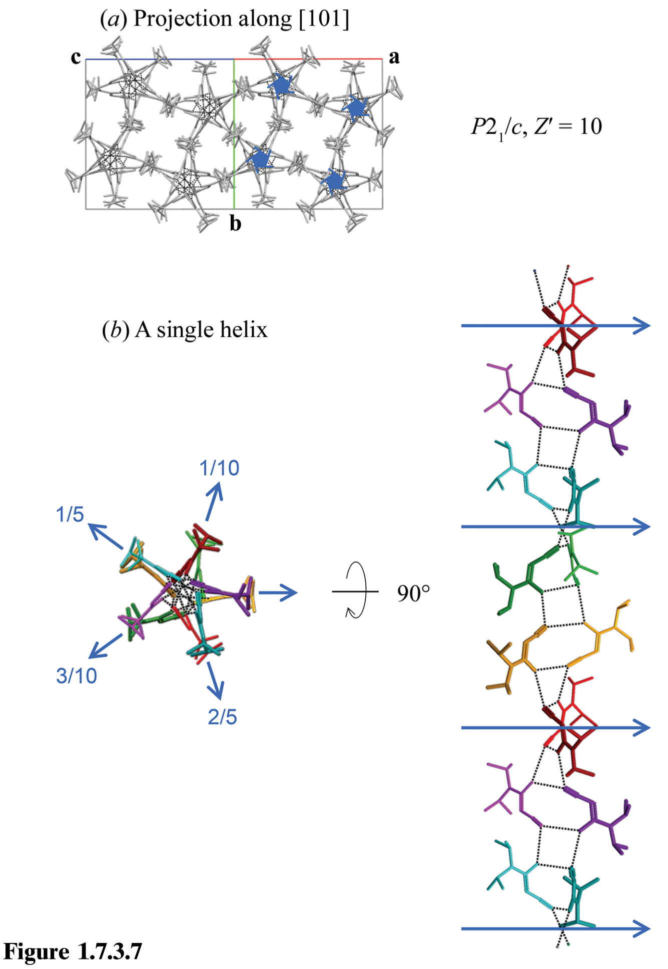

Figure 1.7.3.7
(a) The structure projected along [101] of N''-cyano-N,N-diisopropylguanidine (CSD refcode FEXCAN; Hao *et al.*, 2005; $P2_1/c$, $Z' = 10$). The crystal is composed of fivefold helices; the N(i-Pr)$_2$ groups of adjacent helices are interleaved. (b) Two views of the ten independent molecules in a helix that are linked by NH···NC bonds (H atoms not shown). Each helix has an approximate 5_1 (or 5_4) axis and approximate perpendicular twofold axes, not all of which are shown. The approximate rod group is $\not{p}5_112$ (or $\not{p}5_412$). Rod groups having fivefold axes do not appear in *IT* E, which only illustrates groups having n-fold axes, $n = 2, 3, 4, 6$, but these two $n = 5$ groups are analogous to the groups $\not{p}3_112$ (R47) or $\not{p}3_212$ (R48).

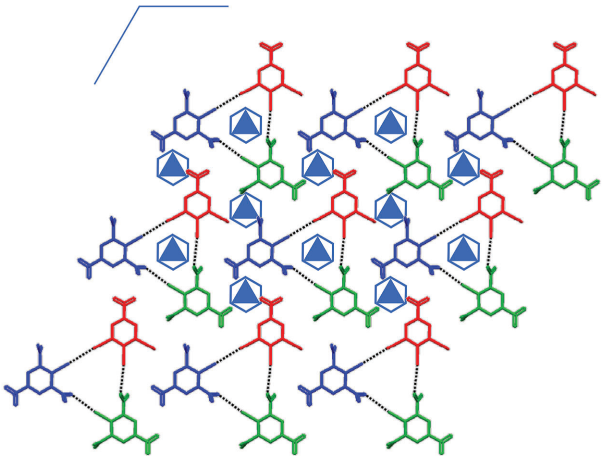

Figure 1.7.3.8
A typical layer (001) in the five polytypes of picryl bromide (CSD refcodes ZZZVXQ0n, $n = 2$–6; Parrish *et al.*, 2008). The space groups are $P1$ ($Z' = 18$), $P\bar{1}$ ($Z' = 6$ and 12), $P3_1$ ($Z' = 12$) and $P6_5$ ($Z' = 3$). The number of independent layers is $Z'/3$, so in the set of polytypes there are 17 independent layers, all of which have approximate symmetry $p\bar{6}$ (L74). The layer angles (γ) for the three triclinic structures are 119.9, 60.2 and 119.9°. The molecules appear to be associated into trimers by Br···O interactions, which are marked.

related by approximate glide planes, twofold axes and 2_1 screw axes. The resulting layer group is $p\bar{4}b2$ (L60), but there are clear deviations from that ideal symmetry; variations in the conformations of the OSiMe$_2$(t-Bu) ring substituent are the most obvious. Those deviations almost certainly arise from interactions between adjacent layers and so might be absent in very small molecular aggregates. In any event, a description using the tetragonal layer group is much more informative than a report of the actual symmetry of an isolated layer, which is only $p1$ (L1).

In the case of a structural rod the approximate symmetry can include, because there is no requirement of periodicity, an n-fold rotation parallel to the rod axis that is not allowed crystallographically; in a one-dimensional rod n can be any positive integer (for a more detailed discussion of rod groups, *cf.* Section 1.7.3.3). Consider the structure with refcode FEXCAN (Hao *et al.*, 2005; Fig. 1.7.3.7). In this monoclinic crystal ten independent molecules form fivefold hydrogen-bonded helices that run along [101]; adjacent helices are in contact in the region of the dimethylamino groups. Half of the helices have approximate $\not{p}5_112$ symmetry; the other half have approximate $\not{p}5_412$ symmetry. *IT* E does not include these two groups because only rod groups with axes allowed in layer and space groups are listed, but all the important features of $\not{p}5_112$ and $\not{p}5_412$ are illustrated by the groups $\not{p}3_112$ (R47) and $\not{p}3_212$ (R48).[5]

In polytypes a single layer type is stacked in different ways to generate a series of polymorphs. While the best known polytypes are inorganic [*e.g.* SiC (Ortiz *et al.*, 2013) and some silicates (Guinier *et al.*, 1984)], molecular polytypes have also been found (*e.g.* 2,4,6-trinitrobromobenzene, ZZZVXQ0n, $n = 2$–6; Parrish *et al.*, 2008). All of the 17 independent layers found in the five ZZZVXQ polytypes are very similar and have approximate layer symmetry $p\bar{6}$ (L74; Fig. 1.7.3.8), although there are deviations from that symmetry, which are most obvious in the rotations of the nitro groups. The symbol $p\bar{6}$ for the approximate layer group is a simple way of summarizing this series of structures.

The examples listed above are all molecular, but subperiodic structural units are perhaps even more common in inorganic structures (see *e.g.* Guinier *et al.*, 1984). Two monolayers of current interest are BN (a graphene analogue) and MoS$_2$ (which contains a central, planar layer of Mo atoms with trigonal prismatic coordination by S atoms). Both monolayers are described by layer group $p\bar{6}m2$ (L78) with both atoms in BN, and the Mo atoms in MoS$_2$, on $\bar{6}m2$ (or D_{3h}) sites, and the S atoms of MoS$_2$ on $3m$ sites (Li, Rao *et al.*, 2013).

1.7.3.3. Applications of rod groups

By Ulrich Müller

When we describe the symmetry of an isolated non-polymeric molecule, we mentally detach it from its surroundings. We even do this when we refer to the molecular structure in a crystal. For example, we say that a molecule of uranocene, U(η^8-C$_8$H$_8$)$_2$, has the point symmetry $8/mmm$ in the crystalline state, even though the molecule actually has only the $\bar{1}$ symmetry required by its site

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[5] *International Tables for Crystallography* defines a screw operation N_q as a counterclockwise rotation of $2\pi/N$ coupled with a fractional translation along the screw axis of $+q/N$ (see Section 1.2.1). The screw axis itself is then right-handed. All pairs of axes N_q and N_{N-q} (*e.g.* 5_1 and 5_4) are enantiomeric. If the screw axis is compatible with space-group symmetry (*e.g.* 3_1, 4_3, 6_2) then the helix is right-handed if $q < N/2$. Note that the handedness of a chemical structure (*i.e.* of a sequence of covalent bonds) may differ from the handedness of the helix generated by the screw axis itself (Müller, 2017); *cf.* Section 1.7.3.3 and Example 3 in that section.

A chemical N/r P or M symbol can be converted to the corresponding Hermann–Mauguin screw axis symbol N_q by the following formula (Alexander, 1969; Spruiell & Clark, 1980):

$$nN \pm 1 = rq,$$

where $n = 0, 1, 2, \ldots$ and $0 < q < N$. The plus sign applies to P helices, the minus sign to M helices. The order N is the same in both symbols. It is not possible to derive the N/r symbol from the Hermann–Mauguin symbol N_q, a unique calculation is not possible (just as the point group of a molecule can be deduced from the molecular structure, but the reverse is impossible). For more details on the symmetry of helical chain molecules see Müller (2017).

If the order of the primary axis of the molecular rod group is $N = 5$ or $N \geq 7$, the order of the primary axis of the penetration rod group can be $N' = 1, 2, 3, 4$ or 6, where N' is a divisor of N. If the primary axis of the molecular rod group is a screw axis N_q, the subscript q' of the screw axis of the penetration group $N'_{q'}$ is the remainder of the integer division $q \div N'$ (Müller, 2017; the axis is a rotation axis if $q' = 0$).

Example 3. The structure of tin iodide phosphide, SnIP, is shown in Fig. 1.7.3.11 (Pfister *et al.*, 2016). It contains polyphosphide ions $(\mathrm{P}^-)_\infty$ that form 7/2 helices. From the formula above we calculate that the helix has a 7_4 screw axis if the helix is chemically right-handed (7/2-P) and 7_3 if it is chemically left-handed (7/2-M). A second 7/2 helix $(\mathrm{SnI}^+)_\infty$ winds around every one of the $(\mathrm{P}^-)_\infty$ helices. The two helices (and also the ensemble of the two helices) have the same screw-axis symmetry. The non-crystallographic molecular rod groups $\not{p}7_421$ and $\not{p}7_321$ describe the symmetries in a nearly perfect way in the racemic crystal (which contains equal numbers of right- and left-handed helices).

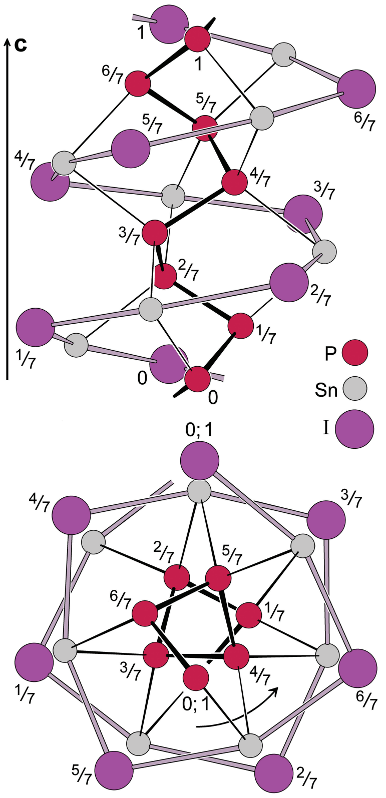


Figure 1.7.3.11
7/2-P helix in SnIP, rod group $\not{p}7_421$. **c** is the translation vector of the molecule. Numbers indicate the heights of the atoms (z coordinates). The curved arrow in the bottom image indicates the pitch of the 7_4 screw axis.

The actual molecular symmetry in the crystal is the penetration rod group $\not{p}121$, which is a subgroup of $\not{p}7_421$ and $\not{p}7_321$ and of the space group $P12/c1$ (No. 13). The crystallographic twofold axes are perpendicular to the helix axis and run through every seventh Sn, I and P atom (at the heights $0, 3.5/7 = \frac{1}{2}$ and 1 in Fig. 1.7.3.11). Whether the connecting Sn–I lines drawn in Fig. 1.7.3.11 are considered to be covalent bonds or not is irrelevant as far as the symmetry is concerned.

1.7.4. Magnetic subperiodic groups and magnetic space groups

By Daniel B. Litvin

1.7.4.1. Introduction

The *magnetic subperiodic groups* in the title of this section refer to generalizations of the crystallographic subperiodic groups, *i.e.* frieze groups (two-dimensional groups with one-dimensional translations), crystallographic rod groups (three-dimensional groups with one-dimensional translations) and layer groups (three-dimensional groups with two-dimensional translations). There are seven frieze-group types, 75 rod-group types and 80 layer-group types, see *IT* E, *Subperiodic Groups* (2010). The magnetic *space groups* refer to generalizations of the one-, two- and three-dimensional crystallographic space groups, n-dimensional groups with n-dimensional translations. There are two one-dimensional space-group types, 17 two-dimensional space-group types and 230 three-dimensional space-group types, see Part 2 of *IT* A.

Generalizations of the crystallographic groups began with the introduction of an operation of 'change in colour' and the 'two-colour' (black and white, antisymmetry) crystallographic point groups (Heesch, 1930; Shubnikov, 1945; Shubnikov *et al.*, 1964). Subperiodic groups and space groups were also extended into two-colour groups. Two-colour subperiodic groups consist of 31 two-colour frieze-group types (Belov, 1956*a*,*b*), 394 two-colour rod-group types (Shubnikov, 1959*a*,*b*; Neronova & Belov, 1961*a*,*b*; Galyarskii & Zamorzaev, 1965*a*,*b*) and 528 two-colour layer-group types (Neronova & Belov, 1961*a*,*b*; Palistrant & Zamorzaev, 1964*a*,*b*). Of the two-colour space groups, there are seven two-colour one-dimensional space-group types (Neronova & Belov, 1961*a*,*b*), 80 two-colour two-dimensional space-group types (Heesch, 1929; Cochran, 1952) and 1651 two-colour three-dimensional space-group types (Zamorzaev, 1953, 1957*a*,*b*; Belov *et al.*, 1957). See also Zamorzaev (1976), Shubnikov & Koptsik (1974), Koptsik (1966, 1967, 1968), and Zamorzaev & Palistrant (1980). [Extensive listings of references on colour symmetry, magnetic symmetry and related topics can be found in the books by Shubnikov *et al.* (1964), Shubnikov & Koptsik (1974), and Opechowski (1986).]

The so-called *magnetic groups*, groups to describe the symmetry of spin arrangements, were introduced by Landau & Lifschitz (1951, 1957) by re-interpreting the operation of 'change in colour' in two-colour crystallographic groups as 'time inversion'. This section introduces the structure, properties and symbols of *magnetic* subperiodic groups and *magnetic* space groups as given in the extensive tables by Litvin (2013), which are an extension of the classic tables of properties of the two- and three-dimensional subperiodic groups found in *IT* E and the one-, two- and three-dimensional space groups found in *IT* A. A survey of magnetic group types is also presented in Litvin

2.1. Guide to and examples of the space-group tables in *IT* A

Theo Hahn, Aafje Looijenga-Vos, Mois I. Aroyo, Howard D. Flack and Koichi Momma

In this chapter, tables and diagrams of crystallographic data for the 17 types of plane groups [Chapter 2.2 of *International Tables for Crystallography* Volume A (2016), hereafter abbreviated as *IT* A] and the 230 types of space groups (Chapter 2.3 of *IT* A) are presented.

Only a minimum of theory is provided here, as the emphasis is on the practical use of the data. For the theoretical background to these data, the reader is referred to Part 1, which also includes suitable references (for further details, see Parts 1 and 3 of *IT* A). A textbook explaining space-group symmetry and the use of the crystallographic data (with exercises) is provided by Hahn & Wondratschek (1994); see also Müller (2013).

Section 2.1.1 displays, with the help of an extensive synoptic table, the classification of the 17 plane groups and 230 space groups. This is followed by an explanation of the characterization of the conventional crystallographic coordinate systems, including the symbols for the centring types of lattices and cells. Section 2.1.2 lists the alphanumeric and graphical symbols for symmetry elements and symmetry operations used throughout *IT* A. The lists are accompanied by notes and cross-references to related IUCr nomenclature reports. Section 2.1.3 explains in a systematic fashion, with many examples and figures, all the entries and diagrams in the order in which they occur in the plane-group and space-group tables of Part 2 of *IT* A. Finally, Section 2.1.4 contains a selection of plane- and space-group tables from *IT* A.

2.1.1. Conventional descriptions of plane and space groups

By Theo Hahn and Aafje Looijenga-Vos

2.1.1.1. Classification of space groups

In *IT* A, the plane groups and space groups are classified according to three criteria:

(i) According to *geometric crystal classes*, *i.e.* according to the crystallographic point group to which a particular space group belongs. There are 10 crystal classes in two dimensions and 32 in three dimensions. They are listed in column 4 of Table 2.1.1.1 (see Chapter 3.2 of *IT* A for a detailed description).

(ii) According to *crystal families*. The term crystal family designates the classification of the 17 plane groups into four categories and of the 230 space groups into *six* categories, as displayed in column 1 of Table 2.1.1.1. Here all 'hexagonal', 'trigonal' and 'rhombohedral' space groups are contained in one family, the hexagonal crystal family. The 'crystal family' thus corresponds to the term 'crystal system', as used frequently in the American and Russian literature.

The crystal families are symbolized by the lower-case letters *a*, *m*, *o*, *t*, *h*, *c*, as listed in column 2 of Table 2.1.1.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Table 2.1.1.2), symbols for the 14 Bravais lattices result. These symbols and their occurrence in the crystal families are shown in column 8 of Table 2.1.1.1; *mS* and *oS* are the standard setting-independent symbols for the centred monoclinic and the one-face-centred orthorhombic Bravais lattices, *cf.* de Wolff *et al.* (1985); symbols between parentheses represent alternative settings of these Bravais lattices.

(iii) According to *crystal systems*. This classification collects the plane groups into four categories and the space groups into *seven* categories. The classifications according to crystal families and crystal systems are the same for two dimensions.

For three dimensions, this applies to the triclinic, monoclinic, orthorhombic, tetragonal and cubic systems. The only complication exists in the hexagonal crystal family, for which several subdivisions into systems have been proposed in the literature. In *IT* A [as well as in *International Tables for X-ray Crystallography* (1952), hereafter *IT* (1952), and the subsequent editions of *IT*], the space groups of the hexagonal crystal family are grouped into two 'crystal systems' as follows: all space groups belonging to the five crystal classes 3, $\bar{3}$, 32, 3*m* and $\bar{3}m$, *i.e.* having 3, 3_1, 3_2 or $\bar{3}$ as principal axis, form the *trigonal* crystal system, irrespective of whether the Bravais lattice is *hP* or *hR*; all space groups belonging to the seven crystal classes 6, $\bar{6}$, 6/*m*, 622, 6*mm*, $\bar{6}2m$ and 6/*mmm*, *i.e.* having 6, 6_1, 6_2, 6_3, 6_4, 6_5 or $\bar{6}$ as principal axis, form the *hexagonal* crystal system; here the lattice is always *hP*. The crystal systems, as defined above, are listed in column 3 of Table 2.1.1.1.

A different subdivision of the hexagonal crystal family is in use, mainly in the French literature. It consists of grouping all space groups based on the hexagonal Bravais lattice *hP* (lattice point symmetry 6/*mmm*) into the 'hexagonal' system and all space groups based on the rhombohedral Bravais lattice *hR* (lattice point symmetry $\bar{3}m$) into the 'rhombohedral' system. In Section 1.3.4, these systems are called 'lattice systems'. They were called 'Bravais systems' in earlier editions of *IT* A.

The theoretical background for the classification of space groups is provided in Section 1.3.4.

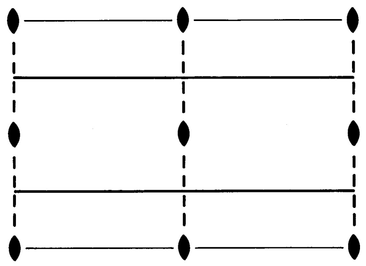
2.1.1.2. Conventional coordinate systems and cells

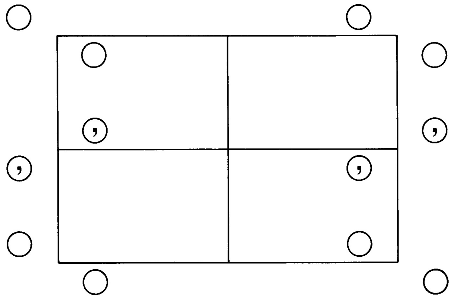
A plane group or space group usually is described by means of a *crystallographic coordinate system*, consisting of a *crystallographic basis* (basis vectors are lattice vectors) and a *crystallographic origin* (origin at a centre of symmetry or at a point of high site symmetry). The choice of such a coordinate system is not mandatory, since in principle a crystal structure can be referred to any coordinate system; *cf.* Chapters 1.3 and 1.5.

The selection of a crystallographic coordinate system is not unique. Conventionally, a right-handed set of basis vectors is taken such that the symmetry of the plane or space group is displayed best. With this convention, which is followed in *IT* A, the specific restrictions imposed on the cell parameters by each crystal family become particularly simple. They are listed in columns 6 and 7 of Table 2.1.1.1. If within these restrictions the smallest cell is chosen, a *conventional* (crystallographic) *basis* results. Together with the selection of an appropriate *conven-*

$p2mg$ $2mm$ Rectangular

No. 7 $p2mg$ Patterson symmetry $p2mm$





Origin at $21g$

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

Symmetry operations

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

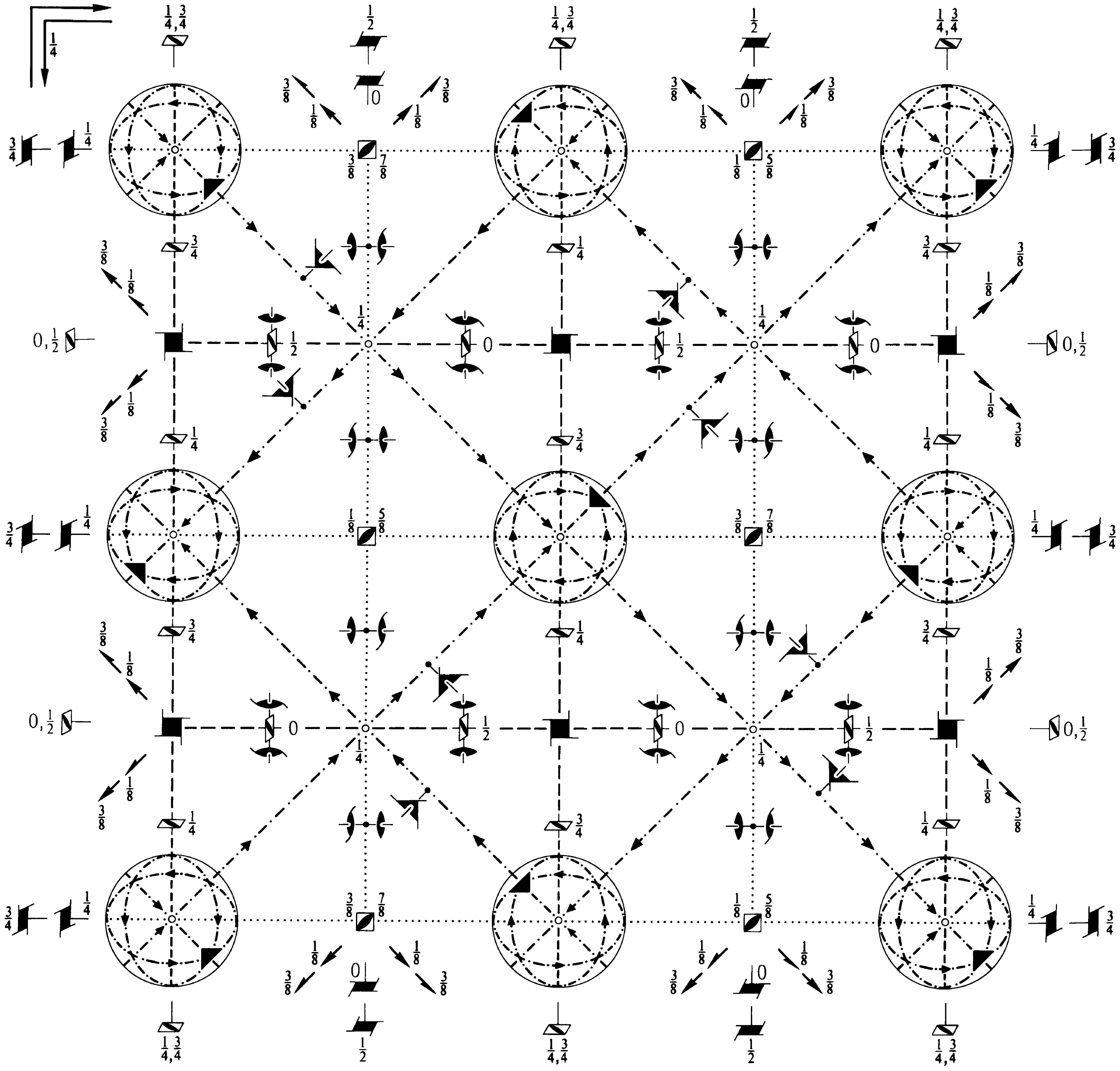
Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

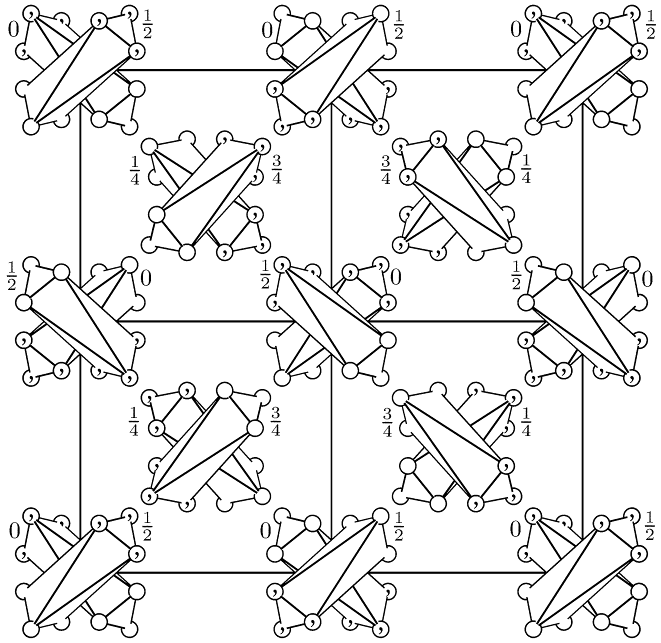
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x}+\frac{1}{2},y$	(4) $x+\frac{1}{2},\bar{y}$	$h0$: $h=2n$
							Special: as above, plus
2	c	$.m.$	$\frac{1}{4},y$	$\frac{3}{4},\bar{y}$			no extra conditions
2	b	$2..$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$			hk: $h=2n$
2	a	$2..$	$0,0$	$\frac{1}{2},0$			hk: $h=2n$

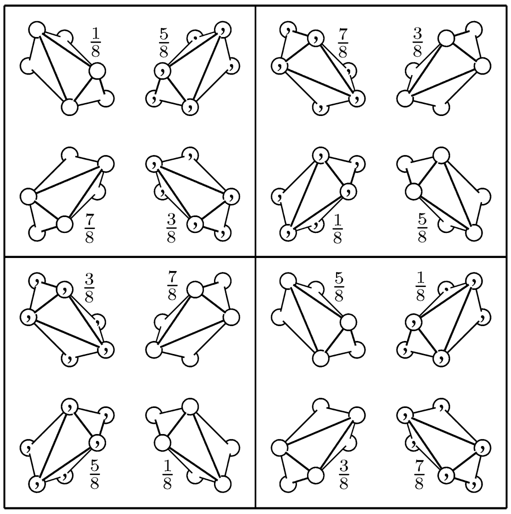
$Ia\bar{3}d$ O_h^{10} $m\bar{3}m$ Cubic

No. 230 $I\ 4_1/a\ \bar{3}\ 2/d$ Patterson symmetry $Im\bar{3}m$





Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$

Origin at centre ($\bar{3}$)

Asymmetric unit $-\frac{1}{8} \le x \le \frac{1}{8}$; $-\frac{1}{8} \le y \le \frac{1}{8}$; $0 \le z \le \frac{1}{4}$; $\max(x,-x,y,-y) \le z$

Vertices $0,0,0$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},-\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{8}$
$\frac{1}{8},\frac{1}{8},\frac{1}{4}$ $-\frac{1}{8},\frac{1}{8},\frac{1}{4}$ $-\frac{1}{8},-\frac{1}{8},\frac{1}{4}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1
(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$
(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(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) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{1}{8}$
(14) $2\quad x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(15) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{4},0,z$
(16) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{3}{4},0,0)\quad x,\frac{1}{4},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{8},y+\frac{1}{4},y$
(19) $2\quad \frac{3}{8},y+\frac{3}{4},\bar{y}$
(20) $4^{+}(\frac{1}{4},0,0)\quad x,-\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{1}{4},0)\quad \frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x-\frac{1}{4},\frac{1}{8},x$
(23) $4^{-}(0,\frac{3}{4},0)\quad 0,y,\frac{1}{4}$
(24) $2\quad \bar{x}+\frac{3}{4},\frac{3}{8},x$
(25) $\bar{1}\quad 0,0,0$
(26) $a\quad x,y,\frac{1}{4}$
(27) $c\quad x,\frac{1}{4},z$
(28) $b\quad \frac{1}{4},y,z$
(29) $\bar{3}^{+}\ x,x,x;\ 0,0,0$
(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$
(31) $\bar{3}^{+}\ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$
(32) $\bar{3}^{+}\ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$
(33) $\bar{3}^{-}\ x,x,x;\ 0,0,0$
(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$
(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$
(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$
(37) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{2},\bar{x},z$
(38) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x,x,z$
(39) $\bar{4}^{-}\ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(40) $\bar{4}^{+}\ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$
(41) $\bar{4}^{-}\ x,0,\frac{3}{4};\ \frac{1}{8},0,\frac{3}{4}$
(42) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{2},\bar{y}$
(43) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x,y,y$
(44) $\bar{4}^{+}\ x,\frac{1}{2},-\frac{1}{4};\ \frac{3}{8},\frac{1}{2},-\frac{1}{4}$
(45) $\bar{4}^{+}\ -\frac{1}{4},y,\frac{1}{2};\ -\frac{1}{4},\frac{3}{8},\frac{1}{2}$
(46) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4})\quad \bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^{-}\ \frac{3}{4},y,0;\ \frac{3}{4},\frac{1}{8},0$
(48) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x,y,x$

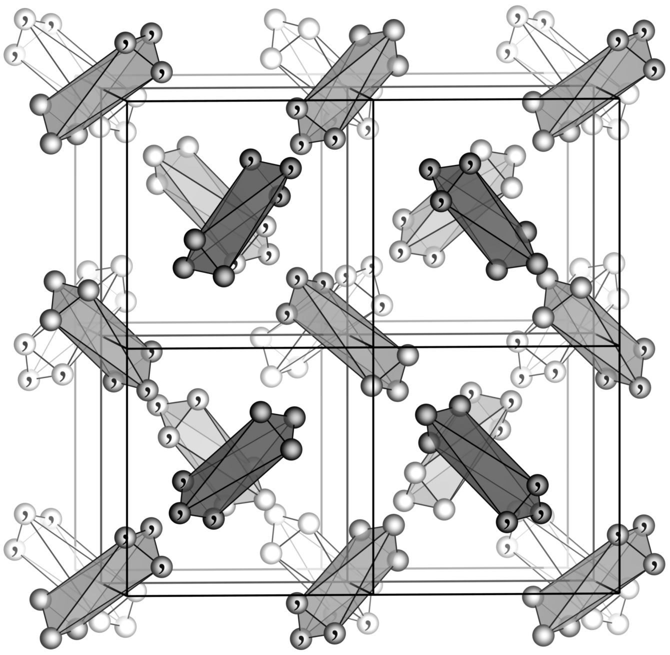
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
(2) $2\quad 0,\frac{1}{4},z$
(3) $2\quad \frac{1}{4},y,0$
(4) $2\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$
(6) $3^{+}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(7) $3^{+}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(8) $3^{+}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^{-}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$
(10) $3^{-}(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^{-}(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^{-}(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{3}{8}$
(14) $2\quad x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^{-}(0,0,\frac{1}{4})\quad \frac{3}{4},0,z$
(16) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{2},z$
(17) $4^{-}(\frac{1}{4},0,0)\quad x,\frac{3}{4},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y-\frac{1}{4},y$
(19) $2\quad \frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^{+}(\frac{3}{4},0,0)\quad x,\frac{1}{4},\frac{1}{2}$
(21) $4^{+}(0,\frac{3}{4},0)\quad \frac{1}{2},y,\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x+\frac{1}{4},\frac{3}{8},x$
(23) $4^{-}(0,\frac{1}{4},0)\quad 0,y,\frac{3}{4}$
(24) $2\quad \bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(26) $b\quad x,y,0$
(27) $a\quad x,0,z$
(28) $c\quad 0,y,z$
(29) $\bar{3}^{+}\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(30) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x,\bar{x};\ -\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(31) $\bar{3}^{+}\ x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ -\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(32) $\bar{3}^{+}\ \bar{x},\bar{x}-\frac{1}{2},x;\ \frac{1}{4},-\frac{1}{4},-\frac{1}{4}$
(33) $\bar{3}^{-}\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(34) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(35) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(36) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(37) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\quad x+\frac{1}{2},\bar{x},z$
(38) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\quad x,x,z$
(39) $\bar{4}^{-}\ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(40) $\bar{4}^{+}\ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$
(41) $\bar{4}^{-}\ x,0,\frac{1}{4};\ \frac{3}{8},0,\frac{1}{4}$
(42) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{2},\bar{y}$
(43) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\quad x,y,y$
(44) $\bar{4}^{+}\ x,\frac{1}{2},\frac{1}{4};\ \frac{1}{8},\frac{1}{2},\frac{1}{4}$
(45) $\bar{4}^{+}\ \frac{1}{4},y,\frac{1}{2};\ \frac{1}{4},\frac{1}{8},\frac{1}{2}$
(46) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad \bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^{-}\ \frac{1}{4},y,0;\ \frac{1}{4},\frac{3}{8},0$
(48) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\quad x,y,x$

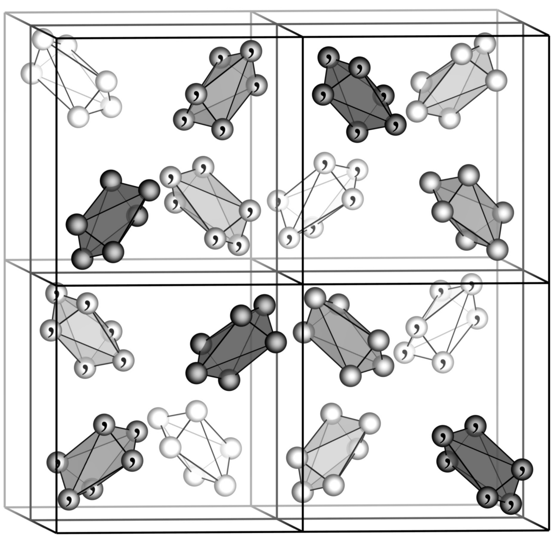
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity,	Wyckoff letter,	Site symmetry	Coordinates								Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$							h,k,l permutable General:
96	h	1	(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) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$					hkl: $h+k+l=2n$
			(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) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$					$0kl$: $k,l=2n$
			(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) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$					hhl: $2h+l=4n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$					$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$					
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$					
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(27) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$					
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(31) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(32) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$					
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(36) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$					
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(38) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(39) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(40) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$					
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(42) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(44) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$					
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(46) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(47) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$					
											Special: as above, plus
48	g	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$					hkl: $h=2n+1$
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$					or $h=4n$
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$					
			$\frac{7}{8},\bar{y},y+\frac{3}{4}$	$\frac{5}{8},y,y+\frac{1}{4}$	$\frac{1}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$					
			$y+\frac{3}{4},\frac{7}{8},\bar{y}$	$y+\frac{1}{4},\frac{5}{8},y$	$\bar{y}+\frac{3}{4},\frac{1}{8},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{3}{8},y+\frac{1}{2}$					
			$\bar{y},y+\frac{3}{4},\frac{7}{8}$	$y,y+\frac{1}{4},\frac{5}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{8}$					
48	f	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$			hkl: $2h+l=4n$
			$\frac{3}{4},x+\frac{1}{4},0$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$	$x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$			
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x},0$	$\frac{1}{4},x+\frac{1}{2},0$	$0,\frac{3}{4},\bar{x}$	$0,\frac{1}{4},x+\frac{1}{2}$			
			$\frac{1}{4},\bar{x}+\frac{3}{4},0$	$\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$x+\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},x+\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\bar{x}+\frac{1}{4}$			
32	e	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$					hkl: $h=2n+1$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$					or $h+k+l=4n$
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$					
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$	$x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$					
24	d	$\bar{4}$ . .	$\frac{3}{8},0,\frac{1}{4}$	$\frac{1}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{3}{8},0$	$\frac{3}{4},\frac{1}{8},0$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{1}{8}$			hkl: $h,k=2n,\ h+k+l=4n$
			$\frac{3}{4},\frac{5}{8},0$	$\frac{3}{4},\frac{3}{8},\frac{1}{2}$	$\frac{1}{8},\frac{1}{2},\frac{1}{4}$	$\frac{7}{8},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{7}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$			or $h,k=2n+1,\ l=4n+2$
24	c	2 . 2 2	$\frac{1}{8},0,\frac{1}{4}$	$\frac{3}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{8},0$	$\frac{3}{4},\frac{3}{8},0$	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$			or $h=8n,\ k=8n+4$ and
			$\frac{7}{8},0,\frac{3}{4}$	$\frac{5}{8},0,\frac{1}{4}$	$\frac{3}{4},\frac{7}{8},0$	$\frac{1}{4},\frac{5}{8},0$	$0,\frac{3}{4},\frac{7}{8}$	$0,\frac{1}{4},\frac{5}{8}$			$h+k+l=4n+2$
16	b	. 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	hkl: $h,k=2n+1,\ l=4n+2$ or $h,k,l=4n$
16	a	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $h,k=2n,\ h+k+l=4n$



Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4}, 0, z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x + \frac{1}{4}, \frac{1}{8}$

2.2. The symmetry-relations tables of *IT* A1

Hans Wondratschek, Mois I. Aroyo and Ulrich Müller

Volume A1 of *International Tables for Crystallography* (2010), referred to as *IT* A1, presents a systematic treatment of the symmetry relations of space groups. For each plane and space group *IT* A1 provides a complete listing of all maximal subgroups and minimal supergroups. There are diagrams of *translationengleiche* and *klassengleiche* subgroups which contain for each space group all kinds of subgroups, not only the maximal ones. These data are complemented by the relations of the Wyckoff positions of the group–maximal subgroup pairs. A short introduction to group–subgroup relations of space groups is given in Chapter 1.7. Here we provide a brief guide to the subgroup tables of *IT* A1 and the related Wyckoff-position relationships; a few representative examples of these tables are included in Sections 2.2.2 and 2.2.4, respectively. For an introduction to and a detailed description of the subgroup data and the Wyckoff-position data, the reader is referred to the corresponding chapters of *IT* A1.

2.2.1. Guide to the subgroup tables

By Hans Wondratschek and Mois I. Aroyo

2.2.1.1. Contents and arrangement of the subgroup tables

In the subgroup tables of *IT* A1 for every space (or plane) group there is a separate table of its maximal subgroups and minimal supergroups. The sequence of the plane groups and space groups $\mathcal{G}$ follows exactly that of the tables of Volume A of *International Tables for Crystallography* (2016), referred to as *IT* A. The listed data consist of the following blocks:

Headline
Generators selected
General position
I Maximal *translationengleiche* subgroups
II Maximal *klassengleiche* subgroups
I Minimal *translationengleiche* supergroups
II Minimal non-isomorphic *klassengleiche* supergroups.

In the *Headline* block the space group whose subgroups are listed is specified by: (i) the *short (international) Hermann–Mauguin* (HM) *symbol* for the space (or plane) group (HM symbols are discussed in Section 1.4.1); (ii) the space- (or plane-) group number as introduced in Vol. I of *International Tables for X-ray Crystallography* (1952); (iii) the *full (international) Hermann–Mauguin symbol* for the space (or plane) group, abbreviated as 'full HM symbol'; and (iv) the *Schoenflies symbol* for the space group (there are no Schoenflies symbols for the plane groups), *cf.* Section 1.4.1.3.

Many of the subgroups $\mathcal{H}$ in these tables are characterized by the elements of their *general position* specified by numbers which refer to the coordinate triplets of the general position of $\mathcal{G}$. Other subgroups are defined by their *generators* specified by numbers which again refer to the general position of $\mathcal{G}$. To ensure the independent use of the tables, the subgroup data for each group $\mathcal{G}$ are preceded by the listings of its general position and the set of generators copied from *IT* A (for a detailed discussion of the general position see Section 1.4.4; for the generators see Section 1.4.3).

In the subgroup tables, depending on their kind, the maximal subgroups are collected under the blocks of *translationengleiche* and *klassengleiche* subgroups.

2.2.1.2. I Maximal *translationengleiche* subgroups (*t*-subgroups)

In this block, all maximal *t*-subgroups $\mathcal{H}$ of the plane and space groups $\mathcal{G}$ are listed individually. The sequence of the subgroups is determined by the rising value of the index and by the decreasing space-group number. For each subgroup $\mathcal{H}$ of index [*i*] in $\mathcal{G}$, the following information is presented in one line:

[*i*] HMS1 (No., HMS2) sequence matrix shift

The symbol HMS1 is the HM symbol of $\mathcal{H}$ referred to the coordinate system and setting of $\mathcal{G}$. The space-group number (No.) of $\mathcal{H}$ and the conventional HM symbol HMS2 of $\mathcal{H}$ if HMS1 is not a conventional one are given in brackets. Each *t*-subgroup $\mathcal{H} < \mathcal{G}$ is defined by its general-position representatives, listed under 'sequence' and specified by numbers, each of which designates an element of $\mathcal{G}$. They are taken from the general position of $\mathcal{G}$ and, therefore, are referred to the coordinate system of $\mathcal{G}$. The matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ for the transformation from the conventional basis of $\mathcal{G}$ to that of $\mathcal{H}$ in concise notation can be read off the columns 'matrix' and 'shift' of the subgroup tables [for details of the concise notation of $(\boldsymbol{P}, \boldsymbol{p})$, see Section 1.5.1.3]. The column 'matrix' is empty if there is no change of basis, *i.e.* if $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$. The column 'shift' is empty if there is no origin shift, *i.e.* if $\boldsymbol{p}$ is the column $\boldsymbol{o}$ consisting of zeroes only.

Conjugate subgroups are listed together and are connected by a left brace.

The way in which the subgroups are described is illustrated by the example of the *t*-subgroups of $P3_112$ (151), *cf.* Section 2.2.2.

I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
[3] $P112$ (5, $C121$)	1; 6	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	0, 0, 1/3
[3] $P112$ (5, $C121$)	1; 5	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	0, 0, 2/3

There are four maximal *t*-subgroups: one trigonal and three conjugate monoclinic subgroups connected by a brace on the left. Note that $P112$ is not the conventional HM symbol for the monoclinic unique axis *c* setting; here, the constituent '2' in the symbols of each of the three subgroups refers to the directions $-2\mathbf{a}-\mathbf{b}$, $\mathbf{a}-\mathbf{b}$ and $\mathbf{a}+2\mathbf{b}$, respectively, in the hexagonal basis. Unique axis *b* is the conventional setting of the monoclinic groups, as expressed by the standard HM symbol $C121$.

The entries in the columns 'matrix' and 'shift' are used for the transformation of matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of the elements of $\mathcal{H}$ to their conventional form. In the case of the trigonal subgroup, these columns are empty because the subgroup is already in the conventional setting, *i.e.* $(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{o})$. The monoclinic subgroups are not in the conventional setting: for

D_3^3 $P3_112$ No. 151 $P3_112$

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

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
			(4) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{1}{3}$	(6) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
[3] $P112$ (5, $C121$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,1/3$
[3] $P112$ (5, $C121$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,2/3$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_212$ (153)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3_212$ (153)	$\langle (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$			
$H3_112$ (152, $P3_121$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3_112$ (152, $P3_121$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3_112$ (152, $P3_121$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3_112$ (152, $P3_121$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$P3_112$ (151)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_112$ (151)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_112$ (151)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_112$ (151)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_212$ (153)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{3}-\frac{2}{3}+2u)\rangle$ prime $p>4$; $0\leq u<p$ p conjugate subgroups for $p=6n-1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P3_112$ (151)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 4+(0,0,\frac{2p}{3}-\frac{2}{3}+2u)\rangle$ prime $p>6$; $0\leq u<p$ p conjugate subgroups for $p=6n+1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P3_112$ (151)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ prime $p\neq 3$; $0\leq u<p$; $0\leq v<p$ p^2 conjugate subgroups	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_122$ (178); [2] $P6_422$ (181)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3_112$ (152, $P3_121$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P312$ (149)

2.2.3. Guide to the tables of relations between Wyckoff positions

By Ulrich Müller

2.2.3.1. Guide to the use of the tables

For an introduction to Wyckoff positions and crystallographic orbits see Section 1.4.4. In Part 3 of *IT* A1, all maximal subgroups of the space groups are listed once again. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given.

The Wyckoff positions are always labelled by their multiplicities and their Wyckoff letters, with the same labels as in the tables of *IT* A and in Section 2.1.4. Reference to *IT* A or to Section 2.1.4 therefore is always necessary, especially when the corresponding coordinate triplets or site symmetries are needed.

The tables in Parts 2 (tables of maximal subgroups) and 3 (relations of the Wyckoff positions) of *IT* A1 and, correspondingly, in Sections 2.2.2 and 2.2.4 deal with different aspects of the reduction of crystal symmetry. Whereas the subject of Part 2 of *IT* A1 is *symmetry*, the subject of Part 3 is the *implications of symmetry changes for crystal structures*. As the subjects of Parts 2 and 3 are different, the presentation of the data in the two parts differs in order to make the listed data as convenient as possible.

Every space group begins on a new page (with the exception of $P4_3$, $P3_2$, $P6_4$ and $P6_5$, which are listed together with $P4_1$, $P3_1$, $P6_2$ and $P6_1$, respectively). If necessary, continuation occurs on the following page(s). The different settings for monoclinic space groups are continued on the same or the following page(s).

The tables are arranged in the following way:

2.2.3.1.1. Headline

The headline lists from the outer margin inwards:

(1) The *short Hermann–Mauguin symbol*;
(2) The number of the space group according to *IT* A;
(3) The *full Hermann–Mauguin symbol* if it differs from the short symbol;
(4) The *Schoenflies symbol*.

In the case of monoclinic space groups, the headline can have one or two additional entries with the full Hermann–Mauguin symbols for different settings.

2.2.3.1.2. Specification of the settings

Each of the monoclinic space groups is listed several times, namely with unique axis *b* and with unique axis *c*, and, if applicable, with the three cell choices 1, 2 and 3 according to *IT* A (see also Section 1.5.4). Space permitting, the entries for the different settings have been combined on one page or on facing pages, since in most cases the Wyckoff-position relations do not depend on the choice of setting. In the few cases where there is a dependence, arrows (⇒) in the corresponding lines show to which settings they refer. Otherwise, the Wyckoff positions of the subgroups correspond to all of the settings listed on the same page or on facing pages.

Rhombohedral space groups are listed only in the setting with hexagonal axes with a rhombohedrally centred obverse cell [*i.e.* $\pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$]. However, for cubic space groups, the rhombohedral subgroups are also given with rhombohedral axes.

Settings with different origin choices are taken account of by two separate columns 'Coordinates' with the headings 'origin 1' and 'origin 2'.

2.2.3.1.3. List of Wyckoff positions

Under the column heading 'Wyckoff positions', the complete sequence of the Wyckoff positions of the space group is given by their multiplicities and Wyckoff letters. If necessary, the sequence runs over two or more lines.

2.2.3.1.4. Subgroup data

The subgroups are divided into two sections: **I Maximal *translationengleiche* subgroups** and **II Maximal *klassengleiche* subgroups**. The latter are further subdivided into three blocks:

Loss of centring translations. This block appears only if the space group has a conventionally centred lattice. The centring has been fully or partly lost in the subgroups listed. The size of the conventional unit cell is not changed.

Enlarged unit cell, non-isomorphic. The *klassengleiche* subgroups listed in this block are non-isomorphic and have conventional unit cells that are enlarged compared with the unit cell of the space group.

Enlarged unit cell, isomorphic. This listing includes the isomorphic subgroups with the smallest possible indices for every kind of cell enlargement. If they exist, index values of 2, 3 and 4 are always given (except for $P\bar{1}$, which is restricted to index 2). If the indices 2, 3 or 4 are not possible, the smallest possible index for the kind of cell enlargement considered is listed. In addition, the infinite series of isomorphic subgroups are given for all possible kinds of cell enlargements. The factor of the cell enlargement corresponds to the index, which is p, p^2 or p^3 (p = prime number; *cf.* Section 2.2.3.1.6). If $p > 2$, the specifically listed subgroups with small index values also always belong to the infinite series, so that the corresponding information is given twice in these cases. For $p = 2$ this applies only to certain special cases.

2.2.3.1.5. Sequence of the listed subgroups

Within each of the aforementioned blocks, the subgroups are listed in the following order. First priority is given to the index, with smallest values first. Subgroups with the same index follow decreasing space-group numbers (according to *IT* A). Exception: the *translationengleiche* subgroup of a tetragonal space group listed last is always the one with the axes transformation to a diagonally oriented cell.

Translationengleiche subgroups of cubic space groups are in the order cubic, rhombohedral, tetragonal, orthorhombic.

In the case of the isomorphic subgroups, there is a subdivision according to the kind of cell enlargement. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements in the direction of the unique axis are given first. For orthorhombic space groups, the isomorphic subgroups with increased **a** are given first, followed by increased **b** and **c**.

The sequence differs somewhat from that in Part 2 of *IT* A1 and Section 2.2.2, where the *klassengleiche* subgroups have been subdivided in more detail according to the different kinds of cell enlargements and the isomorphic subgroups with specific index values have been listed together with the *klassengleiche* subgroups, *i.e.* separately from the infinite series of isomorphic subgroups.

2.2.3.1.6. Information for every subgroup

Index of symmetry reduction

The entry for every subgroup begins with the index of the symmetry reduction in brackets, for example [2] or [p] or [p^2] (p = prime number).

	Axes	Coordinates	Wyckoff positions					
			$2a$ $6g$	$2b$ $6h$	$2c$ $12i$	$2d$ $12j$	$4e$ $12k$	$4f$ $24l$

I Maximal *translationengleiche* subgroups

	Axes	Coordinates	$2a$ / $6g$	$2b$ / $6h$	$2c$ / $12i$	$2d$ / $12j$	$4e$ / $12k$	$4f$ / $24l$
[2] $P\bar{6}2c$ (190)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{6}m2$ (187)		$x,y,z+\frac{1}{4}$	$2g$ $6n$	$1a$; $1b$ $3j$; $3k$	$1d$; $1e$ $12o$	$1c$; $1f$ $6l$; $6m$	$2\times2g$ $2\times6n$	$2h$; $2i$ $2\times12o$
[2] $P6_3mc$ (186)			$2a$ $6c$	$2a$ $6c$	$2b$ $12d$	$2b$ $12d$	$2\times2a$ $2\times6c$	$2\times2b$ $2\times12d$
[2] $P6_322$ (182)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P6_3/m$ (176)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{3}m1$ (164)			$1a$; $1b$ $3e$; $3f$	$2c$ $6i$	$2d$ $6g$; $6h$	$2d$ $12j$	$2\times2c$ $2\times6i$	$2\times2d$ $2\times12j$
[2] $P\bar{3}1c$ (163)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[3] $Cmcm$ (63)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$4a$ $4b$; $8d$	$4c$ $4c$; $8g$	$4c$ $8e$; $16h$	$4c$ $3\times8g$	$8f$ $8f$; $16h$	$8f$ $3\times16h$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$						

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

	Axes	Coordinates	$2a$ / $6g$	$2b$ / $6h$	$2c$ / $12i$	$2d$ / $12j$	$4e$ / $12k$	$4f$ / $24l$
[3] $P6_3/mcm$ (193)	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y)$, z; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	$2b$; $4d$ $6f$; $12i$	$2a$; $4c$ $6g$; $12j$	$6g$ $3\times12i$	$6g$ $3\times12j$	$4e$; $8h$ $12k$; $24l$	$12k$ $3\times24l$

Enlarged unit cell, isomorphic

	Axes	Coordinates	$2a$ / $6g$	$2b$ / $6h$	$2c$ / $12i$	$2d$ / $12j$	$4e$ / $12k$	$4f$ / $24l$
[3] $P6_3/mmc$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$2a$; $4e$ $6g$; $12k$	$2b$; $4e$ $6h$; $12k$	$2d$; $4f$ $12i$; $24l$	$2c$; $4f$ $12j$; $24l$	$3\times4e$ $3\times12k$	$3\times4f$ $3\times24l$
[p] $P6_3/mmc$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2$;	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ $u = 1 \ldots p-1$	$2a$; $\frac{p-1}{2}\times4e$ $6g$; $\frac{p-1}{2}\times12k$	$2b$; $\frac{p-1}{2}\times4e$ $6h$; $\frac{p-1}{2}\times12k$	$2c(d^*)$; $\frac{p-1}{2}\times4f$ $12i$; $\frac{p-1}{2}\times24l$	$2d(c^*)$; $\frac{p-1}{2}\times4f$ $12j$; $\frac{p-1}{2}\times24l$	$p\times4e$ $p\times12k$	$p\times4f$ $p\times24l$
[4] $P6_3/mmc$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2}, 0, 0)$; $+(0, \frac{1}{2}, 0)$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$2a$; $6g$ $12i$; $12k$	$2b$; $6h$ $2\times6h$; $12j$	$2d$; $6h$ $2\times12i$; $24l$	$2c$; $6h$ $4\times12j$	$4e$; $12k$ $2\times12k$; $24l$	$4f$; $12k$ $4\times24l$
[p^2] $P6_3/mmc$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 4$;	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ $u, v = 1, \ldots, p-1$	$2a$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)(p-5)}{12}\times24l$ $6g$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)^2}{4}\times24l$	$2b$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times6h$; $\frac{p(p-1)}{2}\times12j$	$2c(d^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times12i$; $\frac{p(p-1)}{2}\times24l$	$2d(c^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p^2\times12j$	$4e$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p\times12k$; $\frac{p(p-1)}{2}\times24l$	$4f$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p^2\times24l$

$^*\ p = 4n-1$ $^\dagger\ p = 6n-1$

2.3. The subperiodic group tables of *IT* E

Daniel B. Litvin

2.3.1. Guide to the subperiodic group tables

The subperiodic group tables of *International Tables for Crystallography* Volume E (*IT* E, 2010) are an extension of the tables in Volume A, *Space-Group Symmetry* (*IT* A, 2005, 2016). The symmetry tables in *IT* A (2005, 2016) are for the 230 three-dimensional crystallographic space-group types (space groups) and the 17 two-dimensional crystallographic space-group types (plane groups). The analogous symmetry tables in *IT* E (2010) are for the two-dimensional and three-dimensional subperiodic group types: the 7 crystallographic *frieze-group* types (frieze groups, two-dimensional groups with one-dimensional translations), the 75 crystallographic *rod-group* types (rod groups, three-dimensional groups with one-dimensional translations) and the 80 crystallographic *layer-group* types (layer groups, three-dimensional groups with two-dimensional translations).

2.3.1.1. Content and arrangement of the tables

The presentation of the subperiodic group tables follows the form and content of *IT* A (2005). The entries for a subperiodic group are printed on two facing pages or continuously on a single page, where space permits, in the following order:

Left-hand page:

(1) *Headline*;
(2) *Diagrams* for the symmetry elements and the general position;
(3) *Origin*;
(4) *Asymmetric unit*;
(5) *Symmetry operations*.

Right-hand page:

(6) *Headline* in abbreviated form;
(7) *Generators selected*;
(8) General and special *Positions*, with the following columns: *Multiplicity*, *Wyckoff letter*, *Site symmetry*, *Coordinates*, *Reflection conditions*;
(9) *Symmetry of special projections*;
(10) *Maximal non-isotypic non-enantiomorphic subgroups*;
(11) *Maximal isotypic subgroups and enantiomorphic subgroups of lowest index*;
(12) *Minimal non-isotypic non-enantiomorphic supergroups*.

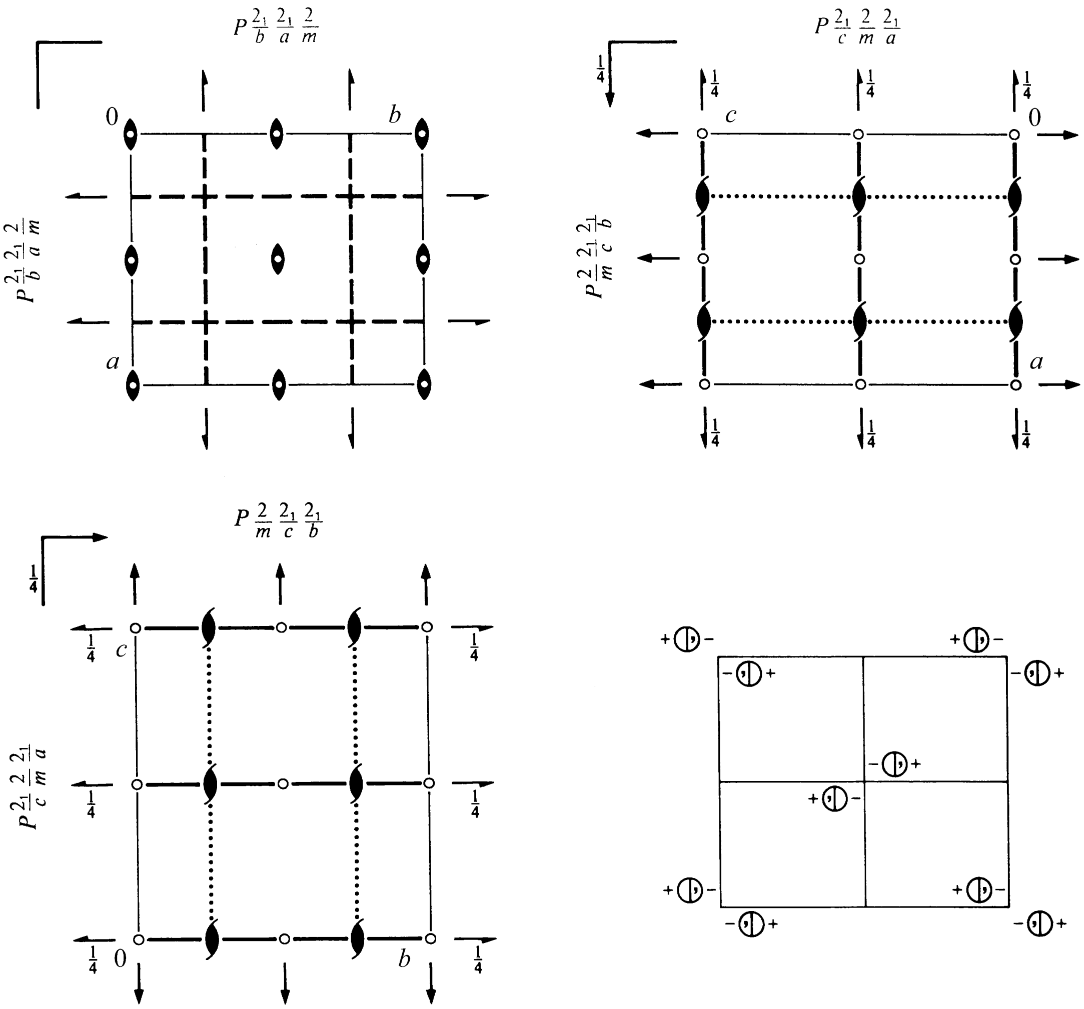
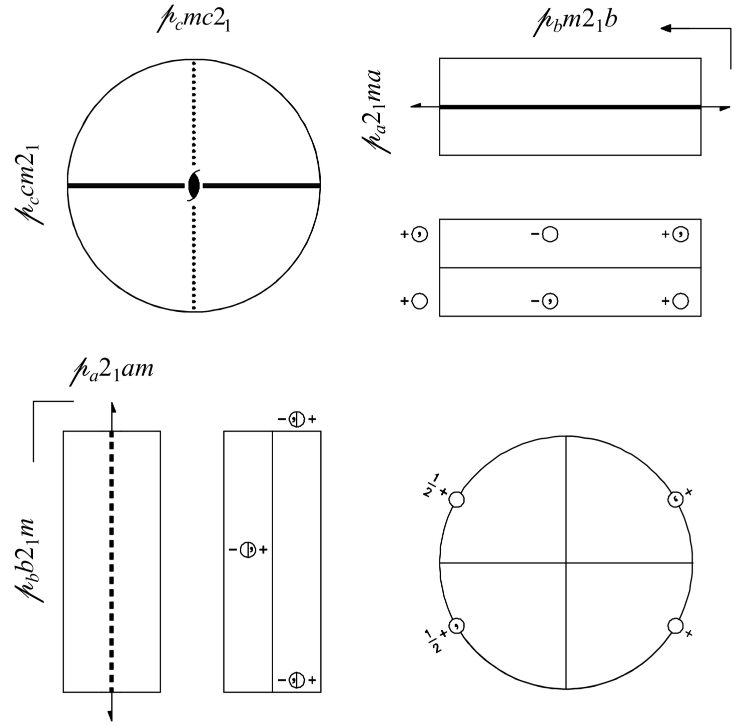


Figure 2.3.1.1
The symmetry-element and general-position diagrams of space group No. 55, *Pbam*.

$\mathscr{p}mc2_1$ $mm2$ Orthorhombic

No. 17 $\mathscr{p}mc2_1$ Patterson symmetry $\mathscr{p}mmm$



Origin on $mc2_1$

Asymmetric unit $0 \leq x$; $0 \leq y$; $0 \leq z \leq 1$

Symmetry operations

(1) 1 $(1|0,0,0)$

(2) $2(\frac{1}{2})$ $0,0,z$ $(2_z|0,0,\frac{1}{2})$

(3) c $x,0,z$ $(m_y|0,0,\frac{1}{2})$

(4) m $0,y,z$ $(m_x|0,0,0)$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	l : $l=2n$
							Special: no extra conditions
2	a	$m\,.\,.$	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $2mm$	Along [100] $\not{p}11g$	Along [010] $\not{p}11m$
	$\mathbf{a}'=\mathbf{c}$	$\mathbf{a}'=\frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $0,y,0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\not{p}112_1$ (9)	1; 2
	$[2]\not{p}1c1$ ($\not{p}c11$, 5)	1; 3
	$[2]\not{p}m11$ (4)	1; 4
IIa	none	
IIb	none	

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\not{p}mc2_1$ ($\mathbf{c}'=3\mathbf{c}$) (17)

Minimal non-isotypic non-enantiomorphic supergroups

I $[2]\not{p}mcm$ (22); $[3]\not{p}6_3mc$ (70)

II $[2]\not{p}mm2$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (15)

2.4. The Symmetry Database

Eli Kroumova, Gemma de la Flor and Mois I. Aroyo

The online edition of *International Tables for Crystallography* at https://it.iucr.org/ includes all the volumes in the series along with the Symmetry Database (https://symmdb.iucr.org/). This database contains more extensive symmetry information for the crystallographic point and space groups than the print editions of *International Tables for Crystallography* Volume A, *Space-Group Symmetry* (2016) (hereafter referred to as *IT* A) or Volume A1, *Symmetry Relations between Space Groups* (2010) (hereafter referred to as *IT* A1). The information in the database can either be retrieved directly from it or generated 'on-the fly' using a range of programs. The different types of data can be accessed through user-friendly menus, and help pages briefly explain the crystallographic data and the functionality of the programs. The data are also presented in different ways, which in some cases includes interactive visualization.

The data and programs that are currently available in the Symmetry Database are arranged into three sections: (i) space-group symmetry data, (ii) symmetry relations between space groups and (iii) 3D crystallographic point groups (*cf.* Fig. 2.4.1.1).

2.4.1. Space-group symmetry data

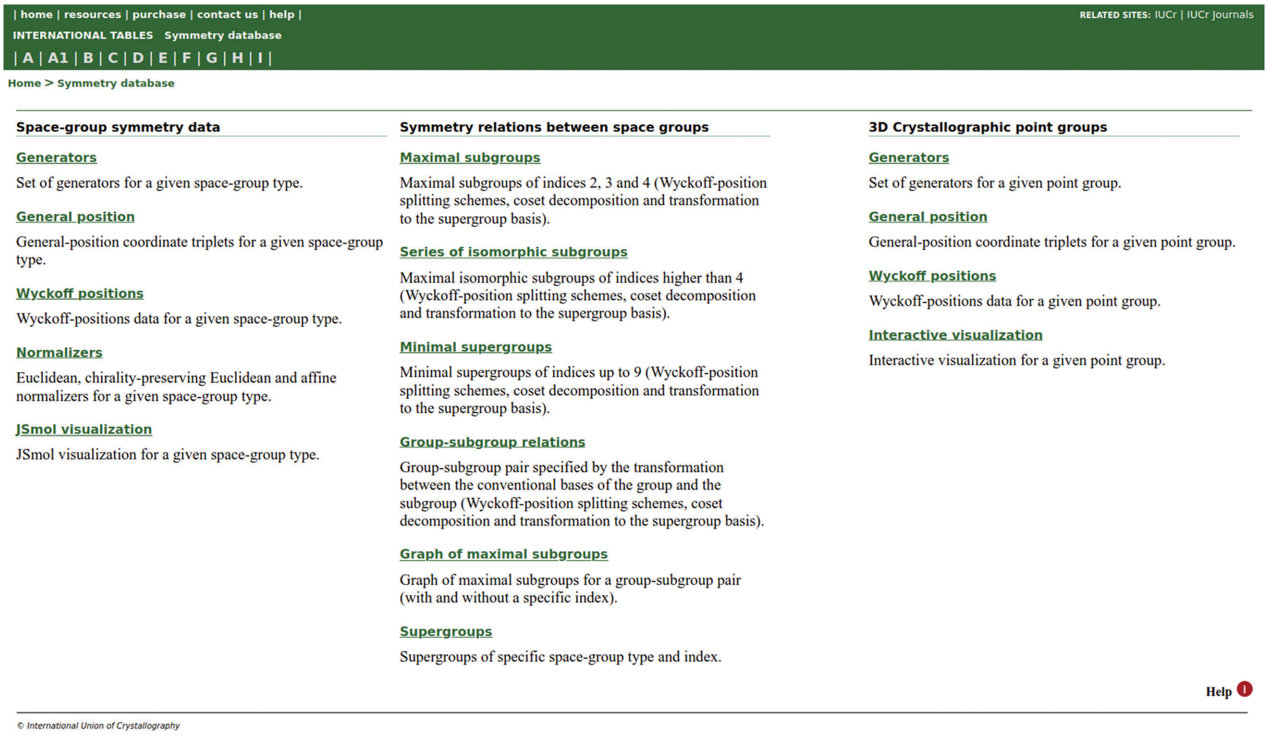
This section hosts crystallographic data for all 230 space groups. Generators (Section 1.4.3), general and special Wyckoff positions (Section 1.4.4), and normalizers (Section 1.1.7) of space groups can be accessed using the appropriately named programs. For all these the user only needs to choose the space group.

The symmetry operations provided by the programs `Generators` and `General position` are presented in four different ways (see Fig. 2.4.1.2): as coordinate triplets, as (3 × 4) matrix–column pairs, using the geometric descriptions that are used in *IT* A (which indicate the type and order of the operations, the location and the orientation of the corresponding geometric elements, and the screw or glide components if relevant) and as Seitz symbols (Section 1.4.2; see also Glazer *et al.*, 2014).

The program `Wyckoff positions` lists the Wyckoff positions for the space group along with their Wyckoff letters and multiplicities, and the oriented symbols of their site-symmetry groups (see Sections 1.4.4 and 2.1.3.12). The coordinate triplets of the points of the Wyckoff position within the unit cell are linked to more detailed information about the corresponding site-symmetry groups. There is also an option for calculating the symmetry operations of the site-symmetry group of any point specified by its coordinates.

These three programs can also provide data for different space-group settings, either by specifying the matrix for the transformation to a new basis (*cf.* Section 1.5.3) or by selecting directly one of the 530 settings listed in Table 1.5.4.4 of *IT* A, all of which are available options.

The program `Normalizers` provides data on the Euclidean, chirality-preserving Euclidean and affine normalizers, which are useful, for example, for comparing descriptions of crystal structures (for more details see Chapter 3.5 of *IT* A). They are described using sets of additional symmetry operations that generate the normalizers successively from the space groups. For triclinic and monoclinic groups whose affine normalizers are not isomorphic to groups of motions, parametric representations of the affine normalizers are shown.



Space-group symmetry data

Generators

Set of generators for a given space-group type.

General position

General-position coordinate triplets for a given space-group type.

Wyckoff positions

Wyckoff-positions data for a given space-group type.

Normalizers

Euclidean, chirality-preserving Euclidean and affine normalizers for a given space-group type.

JSmol visualization

JSmol visualization for a given space-group type.

Symmetry relations between space groups

Maximal subgroups

Maximal subgroups of indices 2, 3 and 4 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis).

Series of isomorphic subgroups

Maximal isomorphic subgroups of indices higher than 4 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis).

Minimal supergroups

Minimal supergroups of indices up to 9 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis).

Group-subgroup relations

Group-subgroup pair specified by the transformation between the conventional bases of the group and the subgroup (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis).

Graph of maximal subgroups

Graph of maximal subgroups for a group-subgroup pair (with and without a specific index).

Supergroups

Supergroups of specific space-group type and index.

3D Crystallographic point groups

Generators

Set of generators for a given point group.

General position

General-position coordinate triplets for a given point group.

Wyckoff positions

Wyckoff-positions data for a given point group.

Interactive visualization

Interactive visualization for a given point group.

Figure 2.4.1.1
Main page of the Symmetry Database for *International Tables for Crystallography*.