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*Volume A*1

SYMMETRY RELATIONS BETWEEN SPACE GROUPS

Edited by

HANS WONDRATSCHEK AND ULRICH MÜLLER

Dedicated to

PAUL NIGGLI AND CARL HERMANN

In 1919, Paul Niggli (1888–1953) published the first compilation of space groups in a form that has been the basis for all later space-group tables, in particular for the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), for *International Tables for X-ray Crystallography* Volume I (1952) and for *International Tables for Crystallography* Volume A (1983). The tables in his book *Geometrische Kristallographie des Diskontinuums* (1919) contained lists of the *Punktlagen*, now known as *Wyckoff positions.* He was a great universal geoscientist, his work covering all fields from crystallography to petrology.

Carl Hermann (1899–1963) published among his seminal works four famous articles in the series *Zur systematischen Strukturtheorie* I to IV in *Z. Kristallogr.* **68** (1928) and **69** (1929). The first article contained the background to the Hermann–Mauguin space-group symbolism. The last article was fundamental to the theory of subgroups of space groups and forms the basis of the maximal-subgroup tables in the present volume. In addition, he was the editor of the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and one of the founders of n-dimensional crystallography, $n > 3$.

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Chapter 1.1 contains a contribution by Professor Y. Billiet, Bourg-Blanc, France, concerning isomorphic subgroups.

Nearly all contributors to this volume, but particularly Professors J. Neubüser and W. Plesken, RWTH Aachen, Germany, and Professor M. I. Aroyo, Universidad del País Vasco, Bilbao, Spain, commented on Chapter 1.2, correcting the text and giving valuable advice. Section 1.2.7 was completely reworked after intensive discussions with Professor V. Janovec, University of Liberec, Czech Republic, making use of his generously offered expertise in the field of domains.

In the late 1960s and early 1970s, J. Neubüser and his team at RWTH Aachen, Germany, calculated the basic lattices of non-isomorphic subgroups by computer. The results now form part of the content of the tables of Chapters 2.2 and 2.3. The team provided a great deal of computer output which was used for the composition of earlier versions of the present tables and for their checking by hand. The typing and checking of the original tables was done with great care and patience by Mrs R. Henke and many other members of the Institut für Kristallographie, Universität Karlsruhe, Germany.

The graphs of Chapters 2.4 and 2.5 were drawn and checked by Professor W. E. Klee, Dr R. Cruse and numerous students and technicians at the Institut für Kristallographie, Universität Karlsruhe, Germany, around 1970. M. I. Aroyo recently rechecked the graphs and transformed the hand-drawn versions into computer graphics.

We are grateful to Dr L. L. Boyle, University of Kent, Canterbury, England, who read, commented on and improved all parts of the text, in particular the English. We thank Professors J. M. Perez-Mato and G. Madariaga, Universidad del País Vasco, Bilbao, Spain, for many helpful discussions on the content and the presentation of the data. M. I. Aroyo would like to note that most of his contribution to this volume was made during his previous appointment in the Faculty of Physics, University of Sofia, Bulgaria, and he is grateful to his former colleagues, especially Drs J. N. Kotzev and M. Mikhov, for their interest and encouragement during this time.

We are indebted to Dr G. Nolze, Bundesanstalt für Materialforschung, Berlin, Germany, for checking the data of Chapter 3.2 using his computer program *POWDER CELL*. We also thank Mrs S. Funke and Mrs H. Sippel, Universität Kassel, Germany, who rechecked a large part of the relations of the Wyckoff positions in this chapter.

Mrs S. E. Barnes, Dr N. J. Ashcroft and the rest of the staff of the International Union of Crystallography in Chester took care of the successful technical production of this volume. In particular, we wish to thank Dr Ashcroft for her tireless help in matters of English style and her guidance in shaping the volume to fit the style of the *International Tables* series.

We gratefully acknowledge the financial support received from various organizations which helped to make this volume possible: in the early stages of the project from the Deutsche Forschungsgemeinschaft, Germany, and more recently from the Alexander von Humboldt-Stiftung, Germany, the International Union for Crystallography, the Sofia University Research Fund, Bulgaria, and the Universidad del País Vasco, Bilbao, Spain.

Contents

Foreword

By Theo Hahn

Symmetry and periodicity are among the most fascinating and characteristic properties of crystals by which they are distinguished from other forms of matter. On the macroscopic level, this symmetry is expressed by point groups, whereas the periodicity is described by translation groups and lattices, and the full structural symmetry of crystals is governed by space groups.

The need for a rigorous treatment of space groups was recognized by crystallographers as early as 1935, when the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* appeared. It was followed in 1952 by Volume I of *International Tables for X-ray Crystallography* and in 1983 by Volume A of *International Tables for Crystallography* (fifth edition 2002). As the depth of experimental and theoretical studies of crystal structures and their properties increased, particularly with regard to comparative crystal chemistry, polymorphism and phase transitions, it became apparent that not only the space group of a given crystal but also its 'descent' and 'ascent', *i.e.* its sub- and supergroups, are of importance and have to be derived and listed.

This had already been done in a small way in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* with the brief inclusion of the *translationengleiche* subgroups of the space groups (see the first volume, pp. 82, 86 and 90). The 1952 edition of *International Tables for X-ray Crystallography* did not contain sub- and supergroups, but in the 1983 edition of *International Tables for Crystallography* the full range of *maximal subgroups* was included (see Volume A, pp. 35–38): *translationengleiche* (type I) and *klassengleiche* (type II), the latter subdivided into 'decentred' (IIa), 'enlarged unit cell' (IIb) and 'isomorphic' (IIc) subgroups. For types I and IIa, *all* subgroups were listed individually, whereas for IIb only the *subgroup types* and for IIc only the *subgroups of lowest index* were given.

All these data were presented in the form known in 1983, and this involved certain omissions and shortcomings in the presentation, *e.g.* no Wyckoff positions of the subgroups and no conjugacy relations were given. Meanwhile, both the theory of subgroups and its application have made considerable progress, and the present Volume A1 is intended to fill the gaps left in Volume A and present the 'complete story' of the sub- and supergroups of space groups in a comprehensive manner. In particular, *all* maximal subgroups of types I, IIa and IIb are listed individually with the appropriate transformation matrices and origin shifts, whereas for the infinitely many maximal subgroups of type IIc expressions are given which contain the complete characterization of all isomorphic subgroups for any given index.

In addition, the relations of the Wyckoff positions for each group–subgroup pair of space groups are listed for the first time in the tables of Part 3 of this volume.

Volume A1 is thus a companion to Volume A, and the editors of both volumes have cooperated closely on problems of symmetry for many years. I wish Volume A1 the same acceptance and success that Volume A has enjoyed.

Scope of this volume

By Mois I. Aroyo, Ulrich Müller and Hans Wondratschek

Group–subgroup relations between space groups, the subject of this volume, are an important tool in crystallographic, physical and chemical investigations. In addition to listing these relations, the corresponding relations between the Wyckoff positions of the group–subgroup pairs are also listed here.

The basis for these tables was laid by the pioneering papers of Carl Hermann in the late 1920s. Some subgroup data were made available in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), together with a graph displaying the symmetry relations between the crystallographic point groups.

Since then, the vast number of crystal structures determined and improvements in experimental physical methods have directed the interest of crystallographers, physicists and chemists to the problems of structure classification and of phase transitions. Methods of computational mathematics have been developed and applied to the problems of crystallographic group theory and group–subgroup relations.

When the new series *International Tables for Crystallography* began to appear in 1983, the subgroup data that were then available were included in Volume A. However, these data were incomplete and their description was only that which was available in the late 1970s. This is still the case in the present (fifth) edition of Volume A.

The subgroup data for the space groups are now complete and form the basis of this volume. After introductory chapters on group-theoretical aspects of space groups, group–subgroup relations between space groups and the underlying mathematical background, this volume provides the reader (in many cases for the first time) with:

(1) complete listings of all maximal non-isomorphic subgroups for each space group, not just by type but individually, including their general positions or their generators, their conjugacy relations and transformations to conventional settings;

(2) listings of the maximal isomorphic subgroups with index 2, 3 or 4 individually in the same way as for non-isomorphic subgroups;

(3) listings of all maximal isomorphic subgroups as members of infinite series, but with the same information as for non-isomorphic subgroups;

(4) data for non-isomorphic supergroups for all space groups (these are already in Volume A) such that the subgroup data may be reversed for problems that involve supergroups of space groups;

(5) two kinds of graphs for all space groups displaying their types of *translationengleiche* subgroups and their types of non-isomorphic *klassengleiche* subgroups;

(6) listings of the splittings of all Wyckoff positions for each space group if its symmetry is reduced to that of a subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained easily from the coordinates in the original space group;

(7) examples explaining how the data in this volume can be used.

The subgroup data in this volume are indispensable for a thorough analysis of phase transitions that do not involve drastic structural changes: the group–subgroup relations indicate the possible symmetry breaks that can occur during a phase transition and they are essential for determining the symmetry of the driving mechanism and the related symmetry of the resulting phase. The group–subgroup graphs describing the symmetry breaks provide information on the possible symmetry modes taking part in the transition and allow a detailed analysis of domain structures and twins. The subgroup relations between the space groups also determine the possible symmetries of intermediate phases that may be involved in the transition pathway in reconstructive phase transitions.

The data in this volume are invaluable for the construction of graphs of group–subgroup relations which visualize in a compact manner the relations between different polymorphic modifications involved in phase transitions and which allow the comparison of crystal structures and their classification into crystal-structure types. Particularly transparent graphs are the family trees that relate crystal structures in the manner developed by Bärnighausen (1980) (also called Bärnighausen trees), which also take into account the relations of the Wyckoff positions of the crystal structures considered. Such family trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases, the possibilities of adapting to different kinds of distortions by reduction of site symmetries and the chemical variations (atomic substitutions) allowed for atomic positions that have become symmetry-independent.

The data on supergroups of space groups are useful for the prediction of high-temperature phase transitions, including the search for new ferroelectric and/or ferroelastic materials, for the treatment of the problem of overlooked symmetry in structure determination and for the study of phase transitions in which a hypothetical parent phase plays an important role.

Computer production of Parts 2 and 3

By Preslav Konstantinov, Asen Kirov, Eli B. Kroumova, Mois I. Aroyo and Ulrich Müller

The text and tables of this volume were produced electronically using the LaTeX 2ε typesetting system (Lamport, 1994), which has the following advantages:

(1) correcting and modifying the text, the layout and the data is easy;

(2) correcting or updating all of the above for future editions of this volume should also be simple;

(3) the cost of production for this first edition and for later editions should be kept low.

At first, sample input files for generating the tables of Part 2 for a few space groups were written which contained LaTeX 2ε instructions for creating both the page layout and the subgroup information. However, these files turned out to be rather complex and difficult to write and to adapt. It proved practically impossible to make changes in the layout. In addition, it could be foreseen that there would be many different layouts for the different space groups. Therefore, this method was abandoned. Instead, a separate data file was created for every space group in each setting listed in the tables. These files contained only the information about the subgroups and supergroups, encoded using specially created LaTeX 2ε commands and macros. These macros were defined in a separate package file which essentially contained the algorithm for the layout. Keeping the formatting information separate from the content as much as possible allowed us to change the layout by redefining the macros without changing the data files. This was done several times during the production of the tables.

The data files are relatively simple and only a minimal knowledge of LaTeX 2ε is required to create and revise them should it be necessary later. A template file was used to facilitate the initial data entry by filling blank spaces and copying pieces of text in a text editor. It was also possible to write computer programs to extract the information from the data files directly. Such programs were used for checking the data in the files that were used to typeset the volume. The data prepared for Part 2 were later converted into a more convenient, machine-readable format so that they could be used in the database of the Bilbao crystallographic server at http://www.cryst.ehu.es/.

The final composition of all plane-group and space-group tables of maximal subgroups and minimal supergroups was done by a single computer job. References in the tables from one page to another were automatically computed. The run takes 1 to 2 minutes on a modern workstation. The result is a PostScript file which can be fed to most laser printers or other modern printing/typesetting equipment.

The resulting files were also used for the preparation of the fifth edition of *International Tables for Crystallography* Volume A (2002) (abbreviated as *IT* A). Sections of the data files of Part 2 of the present volume were transferred directly to the data files for Parts 6 and 7 of *IT* A to provide the subgroup and supergroup information listed there. The formatting macros were rewritten to achieve the layout used in *IT* A.

The different types of data in the LaTeX 2ε files were either keyed by hand or computer-generated. The preparation of the data files of Part 2 can be summarized as follows:

Headline, origin: hand-keyed.

Generators: hand-keyed.

General positions: created by a program from a set of generators. The algorithm uses the well known generating process for space groups based on their solvability property, *cf.* Section 8.3.5 of *IT* A.

Maximal subgroups: hand-keyed. The data for the subgroup generators (or general-position representatives for the cases of *translationengleiche* subgroups and *klassengleiche* subgroups with 'loss of centring translations'), for transformation matrices and for conjugacy relations between subgroups were checked by specially designed computer programs.

Minimal supergroups: created automatically from the data for maximal subgroups.

The electronic preparation of the subgroup tables and the text of Part 2 was carried out on various Unix- and Windows-based computers in Sofia, Bilbao, Stuttgart and Karlsruhe. The development of the computer programs and the layout macros in the package file was done in parallel by different members of the team. Th. Hahn (Aachen) contributed to the final arrangement of the data.

The tables of Part 3 have a different layout, and a style file of their own was created for their production. Again, separate data files were prepared for every space group, containing only the information concerning the subgroups. The macros of the style file were developed by U. Müller, who also hand-keyed all files over the course of seven years.

Most of the data of Part 2 were checked using computer programs developed by F. Gähler (*cf.* Chapter 1.4) and A. Kirov. The relations of the Wyckoff positions (Part 3) were checked by G. Nolze (Berlin) with the aid of his computer program *POWDER CELL* (Nolze, 1996). In addition, all relations were cross-checked with the program *WYCKSPLIT* by Kroumova *et al.* (1998), with the exception of the positions of high multiplicities of some cubic space groups with subgroup indices > 50, which could not be handled by the program.

List of symbols and abbreviations used in this volume

(1) *Points and point space*

P, Q, R	points
O	origin
A_n, $\mathbb{A}_n$, P_n	n-dimensional affine space
E_n, $\mathbb{E}_n$	n-dimensional Euclidean point space
x, y, z; or x_i	point coordinates
$\boldsymbol{x}$	column of point coordinates
$\tilde{X}$	image point
$\tilde{\boldsymbol{x}}$	column of coordinates of an image point
$\tilde{x}_i$	coordinates of an image point
$\boldsymbol{x}'$	column of coordinates in a new coordinate system (after basis transformation)
x'_i	coordinates in a new coordinate system

(2) *Vectors and vector space*

$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$; or $\mathbf{a}_i$	basis vectors of the space
$\mathbf{r}$, $\mathbf{x}$	vectors, position vectors
$\mathbf{o}$	zero vector (all coefficients zero)
a, b, c	lengths of basis vectors } lattice parameters
α, β, γ; or α_j	angles between basis vectors } lattice parameters
$\boldsymbol{r}$	column of vector coefficients
r_i	vector coefficients
$(\mathbf{a})^{\mathrm{T}}$	row of basis vectors
$\mathbf{V}_n$	n-dimensional vector space

(3) *Mappings and their matrices and columns*

$\boldsymbol{A}$, $\boldsymbol{W}$	(3×3) matrices
$\boldsymbol{A}^{\mathrm{T}}$	matrix $\boldsymbol{A}$ transposed
$\boldsymbol{I}$	(3×3) unit matrix
A_{ik}, W_{ik}	matrix coefficients
$(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{W}, \boldsymbol{w})$	matrix–column pairs
$\mathbb{W}$	augmented matrix
$\mathbb{x}$, $\tilde{\mathbb{x}}$, $\mathbb{t}$	augmented columns
$\boldsymbol{P}$, $\mathbb{P}$	transformation matrices
A, I, W	mappings
$\boldsymbol{w}$	column of the translation part of a mapping
w_i	coefficients of the translation part of a mapping
$\boldsymbol{G}$, G_{ik}	fundamental matrix and its coefficients
$\det(\ldots)$	determinant of a matrix
$\mathrm{tr}(\ldots)$	trace of a matrix

(4) *Groups*

$\mathcal{G}$	group; space group
$\mathcal{R}$	space group (Chapter 1.5)
$\mathcal{H}, \mathcal{U}$	subgroups of $\mathcal{G}$
$\mathcal{M}$	maximal subgroup of $\mathcal{G}$ (Chapter 1.5)
$\mathcal{M}$	Hermann's group (Chapter 1.2)
$\mathcal{P}$, $\mathcal{S}$, $\mathcal{V}$, $\mathcal{Z}$	groups
$\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{R})$	group of all translations of $\mathcal{G}$, $\mathcal{R}$
$\mathcal{A}$	group of all affine mappings = affine group
$\mathcal{E}$	group of all isometries (motions) = Euclidean group
$\mathcal{F}$	factor group
$\mathcal{I}$	trivial group, consisting of the unit element e only
$\mathcal{N}$	normal subgroup
$\mathcal{O}$	group of all orthogonal mappings = orthogonal group
$\mathcal{N}_{\mathcal{G}}(\mathcal{H})$	normalizer of $\mathcal{H}$ in $\mathcal{G}$
$\mathcal{N}_{\mathcal{E}}(\mathcal{H})$	Euclidean normalizer of $\mathcal{H}$
$\mathcal{N}_{\mathcal{A}}(\mathcal{H})$	affine normalizer of $\mathcal{H}$
$\mathcal{P}_{\mathcal{G}}$, $\mathcal{P}_{\mathcal{H}}$	point groups of the space groups $\mathcal{G}$, $\mathcal{H}$
$\mathcal{S}_{\mathcal{G}}(X)$, $\mathcal{S}_{\mathcal{H}}(X)$	site-symmetry groups of point X in the space groups $\mathcal{G}$, $\mathcal{H}$
a, b, g, h, m, t	group elements
e	unit element
i or $[i]$	index of $\mathcal{H}$ in $\mathcal{G}$

(5) *Symbols used in the tables*

p	prime number
n, n'	arbitrary positive integer numbers
q, r, u, v, w	arbitrary integer numbers in the given range
$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	basis vectors of the space group
$\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$	basis vectors of the subgroup or supergroup
x, y, z	site coordinates in the space group
$t(1,0,0)$, $t(0,1,0), \ldots$	generating translations

(6) *Abbreviations*

HM symbol	Hermann–Mauguin symbol
IT A	*International Tables for Crystallography* Volume A
PCA	parent-clamping approximation
k-subgroup	*klassengleiche* subgroup
t-subgroup	*translationengleiche* subgroup

SAMPLE PAGES

1.2. General introduction to the subgroups of space groups

BY HANS WONDRATSCHEK

1.2.1. General remarks

The performance of simple vector and matrix calculations, as well as elementary operations with groups, are nowadays common practice in crystallography, especially since computers and suitable programs have become widely available. The authors of this volume therefore assume that the reader has at least some practical experience with matrices and groups and their crystallographic applications. The explanations and definitions of the basic terms of linear algebra and group theory in these first sections of this introduction are accordingly short. Rather than replace an elementary textbook, these first sections aim to acquaint the reader with the method of presentation and the terminology that the authors have chosen for the tables and graphs of this volume. The concepts of groups, their subgroups, isomorphism, coset decomposition and conjugacy are considered to be essential for the use of the tables and for their practical application to crystal structures; for a deeper understanding the concept of normalizers is also necessary. Frequently, however, an 'intuitive feeling' obtained by practical experience may replace a full comprehension of the mathematical meaning. From Section 1.2.6 onwards, the presentation will be more detailed because the subjects are more specialized (but mostly not more difficult) and are seldom found in textbooks.

1.2.2. Mappings and matrices

1.2.2.1. *Crystallographic symmetry operations*

A crystal is a finite block of an infinite periodic array of atoms in physical space. The infinite periodic array is called the *crystal pattern*. The finite block is called the *macroscopic crystal*.

Periodicity implies that there are *translations* which map the crystal pattern onto itself. Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point $\tilde{P}$, the *image point*. The mapping is *reversible* if each image point $\tilde{P}$ is the image of one point P only.

Translations belong to a special category of mappings which leave all distances in the space invariant (and thus within an object and between objects in the space). Furthermore, a mapping of an object onto itself (German: *Deckoperation*) is the basis of the concept of geometric symmetry. This is expressed by the following two definitions.

Definition 1.2.2.1.1. 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 this volume the term 'isometry' is used. □

An isometry is a special kind of affine mapping. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but quotients of lengths on the same line are preserved. In Section 1.2.2.3, the description of affine mappings is discussed, because this type of description also applies to isometries. Affine mappings are important for the classification of crystallographic symmetries, *cf.* Section 1.2.5.2.

Definition 1.2.2.1.2. A mapping is called a *symmetry operation* of an object if

(1) it is an isometry,
(2) it maps the object onto itself. □

Instead of 'maps the object onto itself', one frequently says 'leaves the object invariant (as a whole)'. This does not mean that each point of the object is mapped onto itself; rather, the object is mapped in such a way that an observer cannot distinguish the states of the object before and after the mapping.

Definition 1.2.2.1.3. A symmetry operation of a crystal pattern is called a *crystallographic symmetry operation*. □

The symmetry operations of a macroscopic crystal are also crystallographic symmetry operations, but they belong to another kind of mapping which will be discussed in Section 1.2.5.4.

There are different types of isometries which may be crystallographic symmetry operations. These types are described and discussed in many textbooks of crystallography and in mathematical, physical and chemical textbooks. They are listed here without further treatment. Fixed points are very important for the characterization of isometries.

Definition 1.2.2.1.4. A point P is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{P}$ is the same as the original point P: $\tilde{P} = P$. □

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).

The following kinds of isometries exist:

(1) The *identity operation*, which maps each point of the space onto itself. It is a symmetry operation of every object and, although trivial, is indispensable for the group properties which are discussed in Section 1.2.3.
(2) A *translation* t which shifts every object. A translation is characterized by its translation vector $\mathbf{t}$ and has no fixed point: if $\boldsymbol{x}$ is the column of coordinates of a point P, then the coordinates $\tilde{x}$ of the image point $\tilde{P}$ are $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{t}$. If a translation is a symmetry operation of an object, the object extends infinitely in the directions of $\mathbf{t}$ and $-\mathbf{t}$. A translation preserves the 'handedness' of an object, *e.g.* it maps any right-hand glove onto a right-hand one and any left-hand glove onto a left-hand one.
(3) A *rotation* is an isometry that 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. In particular, a rotation is called an *N-fold rotation* if the rotation angle is $\varphi = k \times 360°/N$, where k and N are relatively prime integers. A rotation preserves the 'handedness' of any object.
(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is now called the *screw axis*. The translation vector is called the *screw vector*. A screw rotation has no fixed points. The screw axis is invariant as a whole under the screw rotation but not pointwise.
(5) An N-fold *rotoinversion* is an N-fold rotation coupled with inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole

1.3. Remarks on Wyckoff positions

BY ULRICH MÜLLER

1.3.1. Introduction

Symmetry relations using crystallographic group–subgroup relations have proved to be a valuable tool in crystal chemistry and crystal physics. Some important applications include :

(1) Structural relations between crystal-structure types can be worked out in a clear and concise manner by setting up family trees of group–subgroup relations (Bärnighausen, 1980; Baur, 1994; Baur & McLarnan, 1982; Bock & Müller, 2002*a*,*b*; Chapuis, 1992; Meyer, 1981; Müller, 1993, 2002; Pöttgen & Hoffmann, 2001).

(2) Elucidation of problems concerning twinned crystals and antiphase domains (*cf.* Section 1.2.7, p. 18; Bärnighausen, 1980; van Tendeloo & Amelinckx, 1974; Wondratschek & Jeitschko, 1976).

(3) Changes of structures and physical properties taking place during phase transitions: applications of Landau theory (Aroyo & Perez-Mato, 1998; Birman, 1966*a*,*b*; Cracknell, 1975; Izyumov & Syromyatnikov, 1990; Landau & Lifshitz, 1980; Salje, 1990; Stokes & Hatch, 1988; Tolédano & Tolédano, 1987).

(4) Prediction of crystal-structure types and calculation of the numbers of possible structure types (McLarnan, 1981*a*,*b*,*c*; Müller, 1978, 1980, 1981, 1986, 1992, 1998, 2003).

All of these applications require consideration of the relations between the atomic sites in a space group and in the corresponding subgroups.

1.3.2. Crystallographic orbits and Wyckoff positions

The set of symmetry-equivalent sites in a space group is referred to as a (*crystallographic point*) *orbit* (Koch & Fischer, 1985; Wondratschek, 1976, 1980, 2002; also called *point configuration*). If the coordinates of a site are completely fixed by symmetry (*e.g.* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$), then the orbit is identical with the corresponding *Wyckoff position* of that space group (in German *Punktlage*). However, if there are one or more freely variable coordinates (*e.g.* z in $0, \frac{1}{2}, z$), the Wyckoff position comprises an infinity of possible orbits; they differ in the values of the variable coordinate(s). The set of sites that are symmetry equivalent to, say, $0, \frac{1}{2}, 0.391$ make up one orbit. The set corresponding to $0, \frac{1}{2}, 0.468$ belongs to the same Wyckoff position, but to another orbit (its variable coordinate z is different).

The Wyckoff positions of the space groups are listed in Volume A of *International Tables for Crystallography* (2002). They are labelled with letters a, b, ..., beginning from the position having the highest site symmetry. A Wyckoff position is usually given together with the number of points belonging to one of its orbits within a unit cell. This number is the *multiplicity* listed in Volume A, and commonly is set in front of the Wyckoff letter. For example, the denomination $4c$ designates the four symmetry-equivalent points belonging to an orbit c within the unit cell.

In many space groups, for some Wyckoff positions there exist several Wyckoff positions of the same kind that can be combined to form a *Wyckoff set* [called a *Konfigurationslage* by Koch & Fischer (1975)]. They have the same site symmetries and they are mapped onto one another by the affine normalizer of the space group (Koch & Fischer, 1975; Wondratschek, 2002).

Example 1.3.2.1.

In space group $I222$, No. 23, there are six Wyckoff positions with the site symmetry 2:

$4e$ $(x, 0, 0)$, $4f$ $(x, 0, \frac{1}{2})$ on twofold rotation axes parallel to **a**,

$4g$ $(0, y, 0)$, $4h$ $(\frac{1}{2}, y, 0)$ on twofold rotation axes parallel to **b**,

$4i$ $(0, 0, z)$, $4j$ $(0, \frac{1}{2}, z)$ on twofold rotation axes parallel to **c**.

They are mapped onto one another by the affine normalizer of $I222$, which is isomorphic to $Pm\overline{3}m$, No. 221. These six Wyckoff positions make up one Wyckoff set.

However, in this example the positions $4e$, $4f$ *vs.* $4g$, $4h$ *vs.* $4i$, $4j$, being on differently oriented axes, cannot be considered to be equivalent if the lattice parameters are $a \neq b \neq c$. The subdivision of the positions of the Wyckoff set into these three sets is accomplished with the aid of the *Euclidean normalizer* of the space group $I222$.

The Euclidean normalizer is that supergroup of a space group that maps all equivalent symmetry elements onto one another without distortions of the lattice. It is a subgroup of the affine normalizer (Fischer & Koch, 1983; Koch *et al.*, 2002). In Example 1.3.2.1 (space group $I222$), the positions $4e$ and $4f$ are equivalent under the Euclidean normalizer (and so are $4g$, $4h$ and also $4i$, $4j$). The Euclidean normalizer of the space group $I222$ is $Pmmm$, No. 47, with the lattice parameters $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$ (if $a \neq b \neq c$). If the origin of a space group is shifted, Wyckoff positions that are equivalent under the Euclidean normalizer may have to be interchanged. The permutations they undergo when the origin is shifted have been listed by Boyle & Lawrenson (1973). An origin shift of $0, 0, \frac{1}{2}$ will interchange the Wyckoff positions $4e$ and $4f$ as well as $4g$ and $4h$ of $I222$.

Example 1.3.2.2.

In the space group $Fm\overline{3}m$, No. 225, the orbits of the Wyckoff positions $4a$ $(0, 0, 0)$ and $4b$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ are equivalent under the Euclidean normalizer. The copper structure can be described equivalently either by having the Cu atoms occupy the position $4a$ or the position $4b$. If we take Cu atoms in the position $4a$ and shift the origin from $(0, 0, 0)$ to $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, then they result in the position $4b$.

Unique relations exist between the Wyckoff positions of a space group and the Wyckoff positions of any of its subgroups (Billiet *et al.*, 1978; Wondratschek, 1993; Wondratschek *et al.*, 1995). Given the relative positions of their unit cells (axes transformations and relative origin positions), the labels of these Wyckoff positions are unique.

Example 1.3.2.3.

In diamond, the carbon atoms occupy the orbit belonging to the Wyckoff position $8a$ of the space group $Fd\overline{3}m$, No. 227. Sphalerite (zinc blende) crystallizes in the maximal subgroup $F\overline{4}3m$, No. 216, of $Fd\overline{3}m$. With the transition $Fd\overline{3}m \to F\overline{4}3m$ the Wyckoff position $8a$ splits into the positions $4a$ and $4c$ of $F\overline{4}3m$.

1.5. The mathematical background of the subgroup tables

By Gabriele Nebe

1.5.1. Introduction

This chapter gives a brief introduction to the mathematics involved in the determination of the subgroups of space groups. To achieve this we have to detach ourselves from the geometric point of view in crystallography and introduce more abstract algebraic structures, such as coordinates, which are well known in crystallography and permit the formalization of symmetry operations, and also the abstract notion of a group, which allows us to apply general theorems to the concrete situation of (three-dimensional) space groups.

This algebraic point of view has the following advantages:

(1) Geometric problems can be treated by algebraic calculations. These calculations can be dealt with by well established procedures. In particular, the use of computers and advanced programs enables one to solve even difficult problems in a comparatively short time.

(2) The mappings form groups in the mathematical sense of the word. This means that the very powerful methods of group theory may be applied successfully.

(3) The procedures for the solution may be developed to a great extent independently of the dimension of the space.

In Section 1.5.2, a basis is laid down which gives the reader an understanding of the algebraic point of view of the crystal space (or point space) and special mappings of this space onto itself. The set of these mappings is an example of a group. For a closer connection to crystallography, the reader may consult Section 8.1.1 of *IT* A (2002) or the book by Hahn & Wondratschek (1994).

Section 1.5.3 gives an introduction to abstract groups and states the important theorems of group theory that will be applied in Section 1.5.4 to the most important groups in crystallography, the space groups. In particular, Section 1.5.4 treats maximal subgroups of space groups which have a special structure by the theorem of Hermann. In Section 1.5.5, we come back to abstract group theory stating general facts about maximal subgroups of groups. These general theorems allow us to calculate the possible indices of maximal subgroups of three-dimensional space groups in Section 1.5.6. The last section, Section 1.5.7, deals with the very subtle question of when these maximal subgroups of a space group are isomorphic to this space group.

1.5.2. The affine space

1.5.2.1. *Motivation*

The aim of this section is to give a mathematical model for the 'point space' (also known in crystallography as 'direct space' or 'crystal space') which the positions of atoms in crystals (the so-called 'points') occupy. This allows us in particular to describe the symmetry groups of crystals and to develop a formalism for calculating with these groups which has the advantage that it works in arbitrary dimensions. Such higher-dimensional spaces up to dimension 6 are used, *e.g.*, for the description of quasicrystals and incommensurate phases. For example, the more than 29 000 000 crystallographic groups up to dimension 6 can be parameterized, constructed and identified using the computer package *[CARAT]: Crystallographic AlgoRithms And Tables*, available from http://wwwb.math.rwth-aachen.de/carat/index.html.

As well as the points in point space, there are other objects, called 'vectors'. The vector that connects the point P to the point Q is usually denoted by $\overrightarrow{PQ}$. Vectors are usually visualized by arrows, where parallel arrows of the same length represent the same vector.

Whereas the sum of two points P and Q is not defined, one can add vectors. The sum $\mathbf{v} + \mathbf{w}$ of two vectors $\mathbf{v}$ and $\mathbf{w}$ is simply the sum of the two arrows. Similarly, multiplication of a vector $\mathbf{v}$ by a real number can be defined.

All the points in point space are equally good, but among the vectors one can be distinguished, the null vector $\mathbf{o}$. It is characterized by the property that $\mathbf{v} + \mathbf{o} = \mathbf{v}$ for all vectors $\mathbf{v}$.

Although the notion of a vector seems to be more complicated than that of a point, we introduce vector spaces before giving a mathematical model for the point space, the so-called affine space, which can be viewed as a certain subset of a higher-dimensional vector space, where the addition of a point and a vector makes sense.

1.5.2.2. *Vector spaces*

We shall now exploit the advantage of being independent of the dimensionality. The following definitions are independent of the dimension by replacing the specific dimensions 2 for the plane and 3 for the space by an unspecified integer number $n > 0$. Although we cannot visualize four- or higher-dimensional objects, we can describe them in such a way that we are able to calculate with such objects and derive their properties.

Algebraically, an n-dimensional (real) vector $\mathbf{v}$ can be represented by a column of n real numbers. The n-dimensional real vector space $\mathbf{V}_n$ is then

$$\mathbf{V}_n = \{\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mid x_1, \ldots, x_n \in \mathbb{R}\}.$$

(In crystallography n is normally 3.) The entries $x_1, \ldots, x_n$ are called the *coefficients* of the vector $\mathbf{x}$. On $\mathbf{V}_n$ one can naturally define an addition, where the coefficients of the sum of two vectors are the corresponding sums of the coefficients of the vectors. To multiply a vector by a real number, one just multiplies all its coefficients by this number. The null vector

$$\mathbf{o} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbf{V}_n$$

can be distinguished, since $\mathbf{v} + \mathbf{o} = \mathbf{v}$ for all $\mathbf{v} \in \mathbf{V}_n$.

The identification of a concrete vector space $\mathbf{V}$ with the vector space $\mathbf{V}_n$ can be done by choosing a basis of $\mathbf{V}$. A *basis* of $\mathbf{V}$ is any tuple of n vectors $\mathbf{B} := (\mathbf{a}_1, \ldots, \mathbf{a}_n)$ such that every vector of $\mathbf{V}$ can be written uniquely as a linear combination of the basis vectors: $\mathbf{V} = \{\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n \mid x_1, \ldots, x_n \in \mathbb{R}\}$. Whereas a vector space has many different bases, the number n of vectors of a basis is uniquely determined and is called the *dimension* of $\mathbf{V}$. The isomorphism (see Section 1.5.3.4 for a definition of isomorphism) $\varphi_{\mathbf{B}}$ between $\mathbf{V}$ and $\mathbf{V}_n$ maps the vector $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n \in \mathbf{V}$

2.1. Guide to the subgroup tables and graphs

By Hans Wondratschek and Mois I. Aroyo

2.1.1. Contents and arrangement of the subgroup tables

In this chapter, the subgroup tables, the subgroup graphs and their general organization are discussed. In the following sections, the different types of data are explained in detail. For every plane group and every space group there is a separate table of maximal subgroups and minimal supergroups. These items are listed either individually, or as members of (infinite) series, or both. In addition, there are graphs of *translationengleiche* and *klassengleiche* subgroups which contain for each space group all kinds of subgroups, not just the maximal ones.

The presentation of the plane-group and space-group data in the tables of Chapters 2.2 and 2.3 follows the style of the tables of Parts 6 (plane groups) and 7 (space groups) in Vol. A of *International Tables for Crystallography* (2002), henceforth abbreviated as *IT* A. The data comprise:

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

For the majority of groups, the data can be listed completely on one page. Sometimes two pages are needed. If the data extend less than half a page over one full page and data for a neighbouring space-group table 'overflow' to a similar extent, then the two overflows are displayed on the same page. Such deviations from the standard sequence are indicated on the relevant pages by a remark *Continued on ...*. The two overflows are separated by a rule and are designated by their headlines.

The sequence of the plane groups and space groups $\mathcal{G}$ in this volume follows exactly that of the tables of Part 6 (plane groups) and Part 7 (space groups) in *IT* A. The format of the subgroup tables has also been chosen to resemble that of the tables of *IT* A as far as possible. Examples of graphs of subgroups can also be found in Section 10.1.4.3 of *IT* A, but only for subgroups of point groups. The graphs for the space groups are described in Section 2.1.7.

2.1.2. Structure of the subgroup tables

Some basic data in these tables have been repeated from the tables of *IT* A in order to allow the use of the subgroup tables independently of *IT* A. These data and the main features of the tables are described in this section. More detailed descriptions are given in the following sections.

2.1.2.1. *Headline*

The headline contains the specification of the space group for which the maximal subgroups are considered. The headline lists from the outside margin inwards:

(1) The *short (international) Hermann–Mauguin symbol* for the plane group or space group. These symbols will be henceforth referred to as 'HM symbols'. HM symbols are discussed in detail in Chapter 12.2 of *IT* A with a brief summary in Section 2.2.4 of *IT* A.

(2) The plane-group or space-group number as introduced in *International Tables for X-ray Crystallography*, Vol. I (1952). These numbers run from 1 to 17 for the plane groups and from 1 to 230 for the space groups.

(3) The *full (international) Hermann–Mauguin symbol* for the plane or space group, abbreviated 'full HM symbol'. This describes the symmetry in up to three symmetry directions (*Blickrichtungen*) more completely, see Table 12.3.4.1 of *IT* A, which also allows comparison with earlier editions of *International Tables*.

(4) The *Schoenflies symbol* for the space group (there are no Schoenflies symbols for the plane groups). The Schoenflies symbols are primarily point-group symbols; they are extended by superscripts for a unique designation of the space-group types, *cf.* *IT* A, Sections 12.1.2 and 12.2.2.

2.1.2.2. *Data from IT A*

2.1.2.2.1. *Generators selected*

As in *IT* A, for each plane group and space group $\mathcal{G}$ a set of symmetry operations is listed under the heading 'Generators selected'. From these group elements, $\mathcal{G}$ can be generated conveniently. The generators in this volume are the same as those in *IT* A. They are explained in Section 2.2.10 of *IT* A and the choice of the generators is explained in Section 8.3.5 of *IT* A.

The generators are listed again in this present volume because many of the subgroups are characterized by their generators. These (often nonconventional) generators of the subgroups can thus be compared with the conventional ones without reference to *IT* A.

2.1.2.2.2. *General position*

Like the generators, the general position has also been copied from *IT* A, where an explanation can be found in Section 2.2.11. The general position in *IT* A is the first block under the heading 'Positions', characterized by its site symmetry of 1. The elements of the general position have the following meanings:

(1) they are coset representatives of the space group $\mathcal{G}$. The other elements of a coset are obtained from its representative by combination with translations of $\mathcal{G}$;

(2) they form a kind of shorthand notation for the matrix description of the coset representatives of $\mathcal{G}$;

(3) they are the coordinates of those symmetry-equivalent points that are obtained by the application of the coset representatives on a point with the coordinates x, y, z;

(4) their numbers refer to the geometric description of the symmetry operations in the block 'Symmetry operations' of the space-group tables of *IT* A.

Many of the subgroups $\mathcal{H}$ in these tables are characterized by the elements of their general position. These elements are specified by numbers which refer to the corresponding numbers in the general position of $\mathcal{G}$. Other subgroups are listed by the numbers of their generators, which again refer to the corresponding numbers in the general position of $\mathcal{G}$. Therefore, the listing of the general position of $\mathcal{G}$ as well as the listing of the generators of $\mathcal{G}$ is essential for empty subblock is then designated by 'none'; in the other subblock the supergroups are listed. The kind of listing depends on the subblock. Examples may be found in the tables of $P222$, No. 16, and $Fd\bar{3}c$, No. 228.

Under the heading 'Additional centring translations', the supergroups are listed by their indices and either by their nonconventional HM symbols, with the space-group numbers and the standard HM symbols in parentheses, or by their conventional HM symbols and only their space-group numbers in parentheses. Examples are provided by space group *Pbca*, No. 61, with both subblocks non-empty and by space group $P222$, No. 16, with supergroups only under the heading 'Additional centring translations'.

Under the heading 'Decreased unit cell' each supergroup is listed by its index and by its lattice relations, where the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$ refer to the supergroup $\mathcal{G}$ and the basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ to the original group $\mathcal{H}$. After these data are listed either the nonconventional HM symbol, followed by the space-group number and the conventional HM symbol in parentheses, or the conventional HM symbol with the space-group number in parentheses. Examples are provided again by space group *Pbca*, No. 61, with both subblocks occupied and space group $F\bar{4}3m$, No. 216, with an empty subblock 'Additional centring translations' but data under the heading 'Decreased unit cell'.

2.1.6.4. *Isomorphic supergroups*

Each space group $\mathcal{G}$ has an infinite number of isomorphic subgroups $\mathcal{H}$ because the number of primes is infinite. For the same reason, each space group $\mathcal{H}$ has an infinite number of isomorphic supergroups $\mathcal{G}$. They are not listed in the tables of this volume because they are implicitly listed among the subgroup data.

2.1.7. The subgroup graphs

2.1.7.1. *General remarks*

The group–subgroup relations between the space groups may also be described by graphs. This way is chosen in Chapters 2.4 and 2.5. Graphs for the group–subgroup relations between crystallographic point groups have been published, for example, in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and in *IT* A (2002), Fig. 10.1.4.3. Three kinds of graphs for subgroups of space groups have been constructed and can be found in the literature:

(1) Graphs for *t*-subgroups, such as the graphs of Ascher (1968).
(2) Graphs for *k*-subgroups, such as the graphs for cubic space groups of Neubüser & Wondratschek (1966).
(3) Mixed graphs, combining *t*- and *k*-subgroups. These are used, for example, when relations between existing or suspected crystal structures are to be displayed. An example is the 'family tree' of Bärnighausen (1980), Fig. 15, now called a *Bärnighausen tree*.

A complete collection of graphs of the first two kinds is presented in this volume: in Chapter 2.4 those displaying the *translationengleiche* or *t*-subgroup relations and in Chapter 2.5 those for the *klassengleiche* or *k*-subgroup relations. Neither type of graph is restricted to maximal subgroups but both contain *t*- or *k*-subgroups of higher indices, with the exception of isomorphic subgroups, *cf.* Section 2.1.7.3 below.

The group–subgroup relations are direct relations between the space groups themselves, not between their types. However, each such relation is valid for a pair of space groups, one from each of the types, and for each space group of a given type there exists a corresponding relation. In this sense, one can speak of a relation between the space-group types, keeping in mind the difference between space groups and space-group types, *cf.* Section 1.2.5.3.

The space groups in the graphs are denoted by the standard HM symbols and the space-group numbers. In each graph, each space-group type is displayed at most once. Such graphs are called *contracted graphs* here. Without this contraction, the more complex graphs would be much too large for the page size of this volume.

The symbol of a space group $\mathcal{G}$ is connected by uninterrupted straight lines with the symbols of all maximal non-isomorphic subgroups $\mathcal{H}$ or minimal non-isomorphic supergroups $\mathcal{S}$ of $\mathcal{G}$. In general, the *maximal subgroups* of $\mathcal{G}$ are drawn on a *lower level* than $\mathcal{G}$; in the same way, the *minimal supergroups* of $\mathcal{G}$ are mostly drawn on a *higher level* than $\mathcal{G}$. For exceptions see Section 2.1.7.3. Multiple lines may occur in the graphs for *t*-subgroups. They are explained in Section 2.1.7.2. No indices are attached to the lines. They can be taken from the corresponding subgroup tables of Chapter 2.3, and are also provided by the general formulae of Section 1.2.8. For the *k*-subgroup graphs, they are further specified at the end of Section 2.1.7.3.

2.1.7.2. *Graphs for translationengleiche subgroups*

Let $\mathcal{G}$ be a space group and $\mathcal{T}(\mathcal{G})$ the normal subgroup of all its translations. Owing to the isomorphism between the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ and the point group $\mathcal{P}_{\mathcal{G}}$, see Section 1.2.5.4, according to the first isomorphism theorem, Ledermann (1976), *t*-subgroup graphs are the same (up to the symbols) as the corresponding graphs between point groups. However, in this volume, the graphs are not complete but are contracted by displaying each space-group type at most once. This contraction may cause the graphs to look different from the point-group graphs and also different for different space groups of the same point group, *cf.* Example 2.1.7.2.1.

One can indicate the connections between a space group $\mathcal{G}$ and its maximal subgroups in different ways. In the contracted *t*-subgroup graphs one line is drawn for each conjugacy class of maximal subgroups of $\mathcal{G}$. Thus, a line represents the connection to an individual subgroup only if this is a normal maximal subgroup of $\mathcal{G}$, otherwise it represents the connection to more than one subgroup. The conjugacy relations are not necessarily transferable to non-maximal subgroups, *cf.* Example 2.1.7.2.2. On the other hand, multiple lines are possible, see the examples. Although it is not in general possible to reconstruct the complete graph from the contracted one, the content of information of such a graph is higher than that of a graph which is drawn with simple lines only.

The graph for the space group at its top also contains the contracted graphs for all subgroups which occur in it, see the remark below Example 2.1.7.2.2.

Owing to lack of space for the large graphs, in all graphs of *t*-subgroups the group $P1$, No. 1, and its connections have been omitted. Therefore, to obtain the full graph one has to supplement the graphs by $P1$ at the bottom and to connect $P1$ by one line to each of the symbols that have no connection downwards.

Within the same graph, symbols on the same level indicate subgroups of the same index relative to the group at the top. The distance between the levels indicates the size of the index. For a more detailed discussion, see Example 2.1.7.2.2. For the sequence and the numbers of the graphs, see the paragraph below Example 2.1.7.2.2.

$p2mg$ No. 7 $p2mg$

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

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x}+\frac{1}{2},y$ (4) $x+\frac{1}{2},\bar{y}$

I Maximal *translationengleiche* subgroups

[2] $p11g$ (4, pg)	1; 4	$-\mathbf{b},\mathbf{a}$	
[2] $p1m1$ (3, pm)	1; 3		$1/4,0$
[2] $p211$ (2, $p2$)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$p2gg$ (8)	$\langle 2;\ 3+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	
$p2gg$ (8)	$\langle (2;\ 3)+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	$0,1/2$
$p2mg$ (7)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b}$	
$p2mg$ (7)	$\langle 3;\ 2+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	$0,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$p2mg$ (7)	$\langle 2;\ 3+(1,0)\rangle$	$3\mathbf{a},\mathbf{b}$	
$p2mg$ (7)	$\langle 2+(2,0);\ 3+(3,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
$p2mg$ (7)	$\langle 2+(4,0);\ 3+(5,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$p2mg$ (7)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b}$	
$p2mg$ (7)	$\langle 3;\ 2+(0,2)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,1$
$p2mg$ (7)	$\langle 3;\ 2+(0,4)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$p2mg$ (7)	$\langle 2+(2u,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$p2mg$ (7)	$\langle 3;\ 2+(0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b}$	$0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $c2mm$ (9)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $p2mm$ (6)

Cm No. 8 $A11m$ C_s^3

UNIQUE AXIS c, CELL CHOICE 1

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

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$
4	b	1	(1) x,y,z (2) $x,y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $A1$ (1, $P1$)	1+	$\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P11b$ (7, $P11a$)	1; $2+(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,1/4$
[2] $P11m$ (6)	1; 2		

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$A11a$ (9)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$I11a$ (9, $A11a$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$A11m$ (8)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$I11m$ (8, $A11m$)	$\langle 2\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $A11m$ (8)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $A11m$ (8)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $A11m$ (8)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	
[3] $\mathbf{b}'=3\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$A11m$ (8)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$ $p>1$; $0\le q<p$ no conjugate subgroups	$p\mathbf{a},-2q\mathbf{a}+\mathbf{b},\mathbf{c}$	
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $A112/m$ (12); [2] $Cmm2$ (35); [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Fmm2$ (42); [2] $Imm2$ (44); [2] $Ima2$ (46); [3] $P3m1$ (156); [3] $P31m$ (157); [3] $R3m$ (160)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P11m$ (6)

$Ibam$ No. 72 $I2/b2/a2/m$ D_{2h}^{26}

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)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Ib2m$ (46, $Ima2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $I2am$ (46, $Ima2$)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,0,1/4$
[2] $Iba2$ (45)	(1; 2; 7; 8)+		
[2] $I222$ (23)	(1; 2; 3; 4)+		$0,0,1/4$
[2] $I12/a1$ (15, $C12/c1$)	(1; 3; 5; 7)+	$\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{c}$	
[2] $I2/b11$ (15, $C12/c1$)	(1; 4; 5; 8)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	
[2] $I112/m$ (12, $A112/m$)	(1; 2; 5; 6)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pcan$ (60, $Pbcn$)	1; 3; 5; 7; (2; 4; 6; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pbcn$ (60)	1; 4; 5; 8; (2; 3; 6; 7) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pbcm$ (57)	1; 3; 6; 8; (2; 4; 5; 7) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $Pcam$ (57, $Pbcm$)	1; 4; 6; 7; (2; 3; 5; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,1/4$
[2] $Pccn$ (56)	1; 2; 3; 4; (5; 6; 7; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $Pbam$ (55)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pban$ (50)	1; 2; 7; 8; (3; 4; 5; 6) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $Pccm$ (49)	1; 2; 5; 6; (3; 4; 7; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Ibam$ (72)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ibam$ (72)	$\langle(2;\ 5)+(2,0,0);\ 3+(3,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Ibam$ (72)	$\langle(2;\ 5)+(4,0,0);\ 3+(5,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Ibam$ (72)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Ibam$ (72)	$\langle(2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Ibam$ (72)	$\langle(2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Ibam$ (72)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Ibam$ (72)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Ibam$ (72)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Ibam$ (72)	$\langle(2;\ 5)+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Ibam$ (72)	$\langle(2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Ibam$ (72)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $I4/mcm$ (140)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmmm$ (65); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Aemm$ (67, $Cmme$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Bmem$ (67, $Cmme$)

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

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	h	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $y,\bar{x},\bar{z}$ (4) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P2$ (3, $P112$) 1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3 \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,1) \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C\bar{4}$ (81, $P\bar{4}$)	$\langle 2;\ 3 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}$ (81, $P\bar{4}$)	$\langle 2+(1,1,0);\ 3+(0,1,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F\bar{4}$ (82, $I\bar{4}$)	$\langle 2;\ 3 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}$ (82, $I\bar{4}$)	$\langle 2;\ 3+(0,0,1) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,4) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,2u) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P\bar{4}$ (81)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0) \rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p = q^2 + r^2$] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b},\ \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$			
$P\bar{4}$ (81)	$\langle 2+(2u,0,0);\ 3+(u,u,0) \rangle$ $q > 0;\ r > 0;\ p > 4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/m$ (83); [2] $P4_2/m$ (84); [2] $P4/n$ (85); [2] $P4_2/n$ (86); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I\bar{4}$ (82)

- **Decreased unit cell** none

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	e	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P1m1$ (8, $C1m1$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P1m1$ (8, $C1m1$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P1m1$ (8, $C1m1$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3c1$ (158)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3m1$ (157, $P31m$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3m1$ (157, $P31m$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3m1$ (157, $P31m$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3m1$ (157, $P31m$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3m1$ (156)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3m1$ (156)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3m1$ (156)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3m1$ (156)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}m1$ (164); [2] $P6mm$ (183); [2] $P6_3mc$ (186); [2] $P\bar{6}m2$ (187)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3m1$ (157, $P31m$); [3] $R_{\text{obv}}3m$ (160, $R3m$); [3] $R_{\text{rev}}3m$ (160, $R3m$)

- **Decreased unit cell** none

ORIGIN CHOICE 1, Origin at 432, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre $(\bar{3})$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
48	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/4,1/4,1/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$3/4,1/4,3/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/4,3/4,3/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$3/4,3/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}n$ (222)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(u-v,-u+v,2w);$ $25+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,\frac{p}{2}-\frac{1}{2}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

- **Decreased unit cell** none

$Pn\bar{3}n$ No. 222 $P4/n\bar{3}2/n$ O_h^2

ORIGIN CHOICE 2, Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 432

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
48 i 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
	(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
	(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
	(13) $y,x,\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y,\bar{x}+\frac{1}{2},z$	(16) $\bar{y}+\frac{1}{2},x,z$
	(17) $x,z,\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z,y$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x,\bar{z}+\frac{1}{2},y$
	(21) $z,y,\bar{x}+\frac{1}{2}$	(22) $z,\bar{y}+\frac{1}{2},x$	(23) $\bar{z}+\frac{1}{2},y,x$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
	(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
	(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$
	(37) $\bar{y},\bar{x},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y},x+\frac{1}{2},\bar{z}$	(40) $y+\frac{1}{2},\bar{x},\bar{z}$
	(41) $\bar{x},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z},\bar{y}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x},z+\frac{1}{2},\bar{y}$
	(45) $\bar{z},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}$	(47) $z+\frac{1}{2},\bar{y},\bar{x}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		$1/4,1/4,1/4$
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		$1/4,1/4,1/4$
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$1/2,0,1/2$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$0,1/2,1/2$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$1/2,1/2,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}n$ (222)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(\frac{p}{2}-\frac{1}{2}+2u,0,\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(u-v,-u+v,\frac{p}{2}-\frac{1}{2}+2w)$; $25+(2u,2v,2w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

- **Decreased unit cell** none

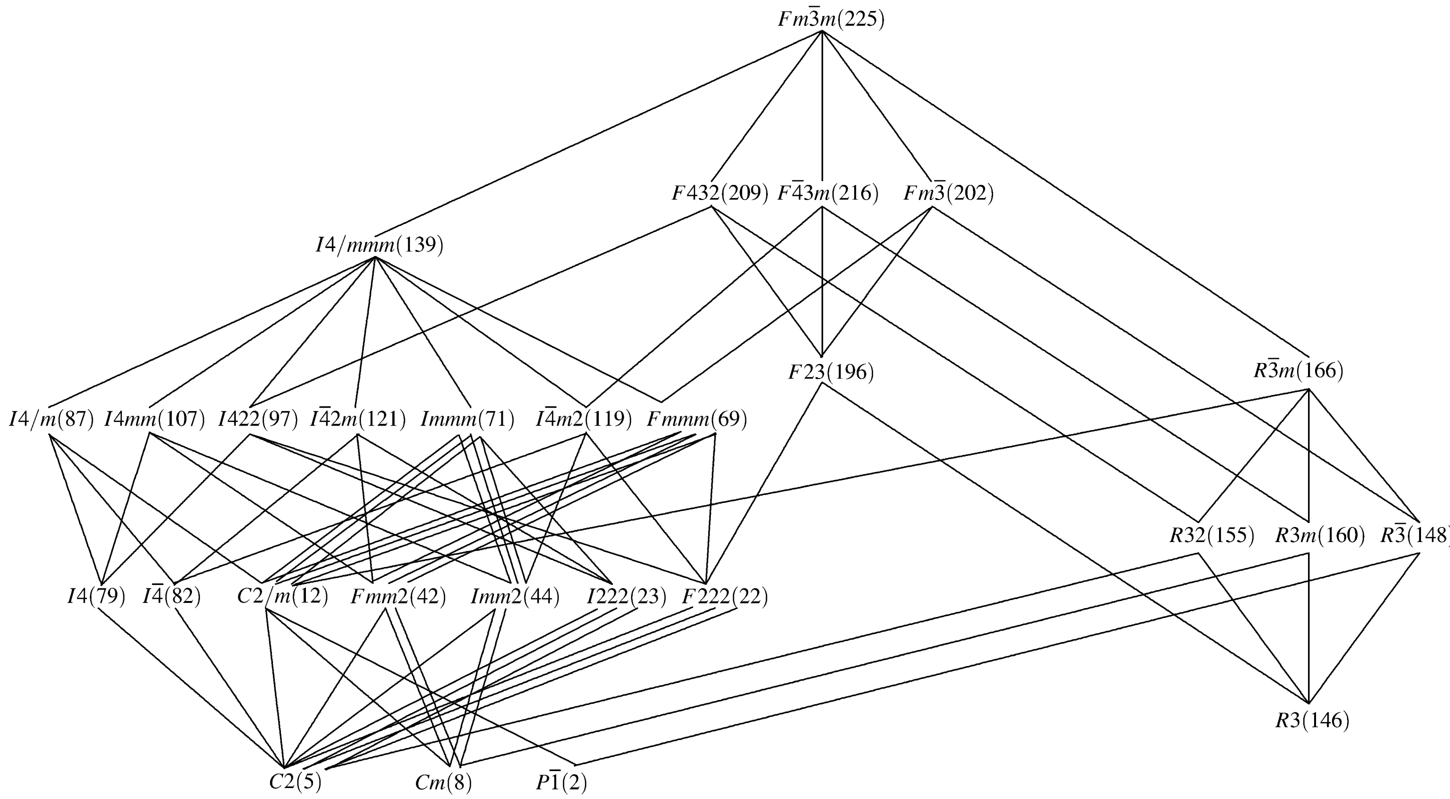

Fig. 2.4.1.5. Graph of the *translationengleiche* subgroups of the space group $Fm\bar{3}m$.

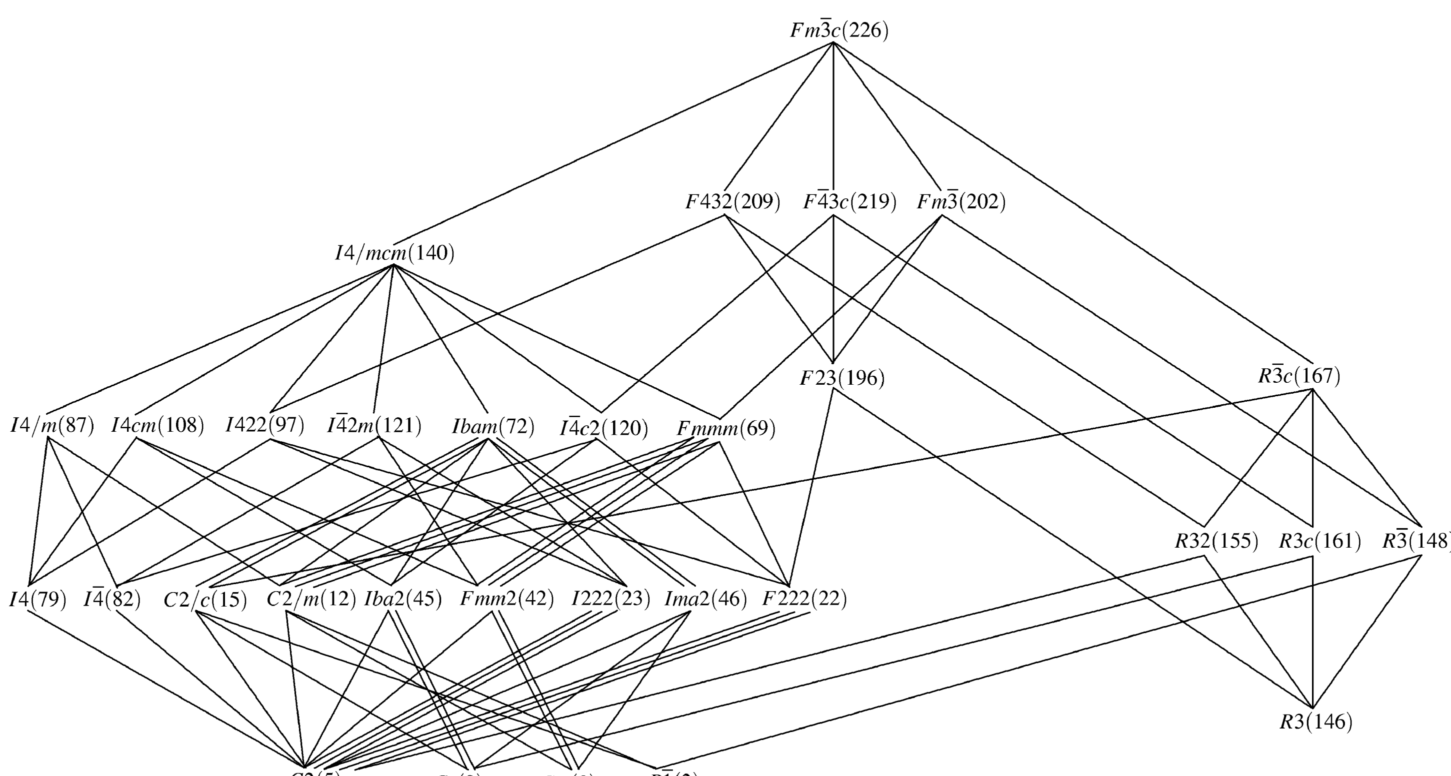

Fig. 2.4.1.6. Graph of the *translationengleiche* subgroups of the space group $Fm\bar{3}c$.

2.5.3. Graphs of the *klassengleiche* subgroups of trigonal space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

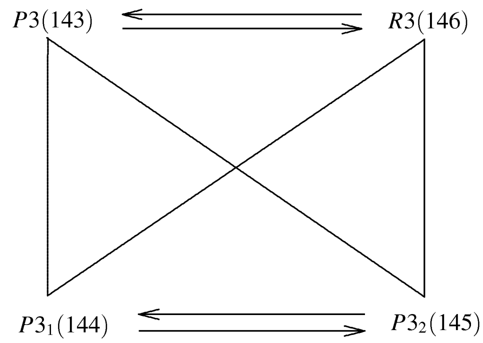

Fig. 2.5.3.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 3.

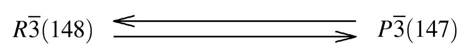

Fig. 2.5.3.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\overline{3}$.

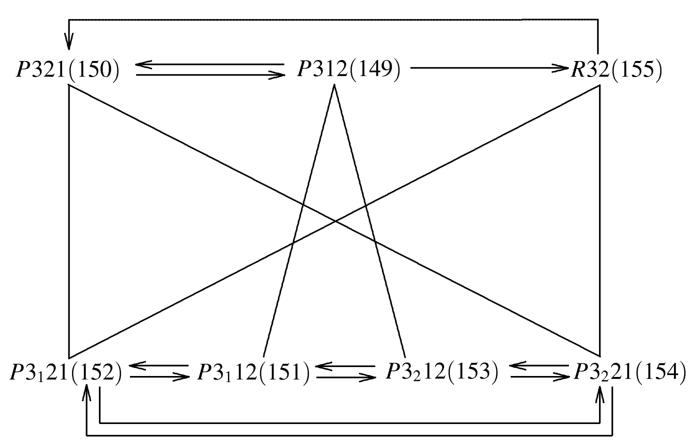

Fig. 2.5.3.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class 32.

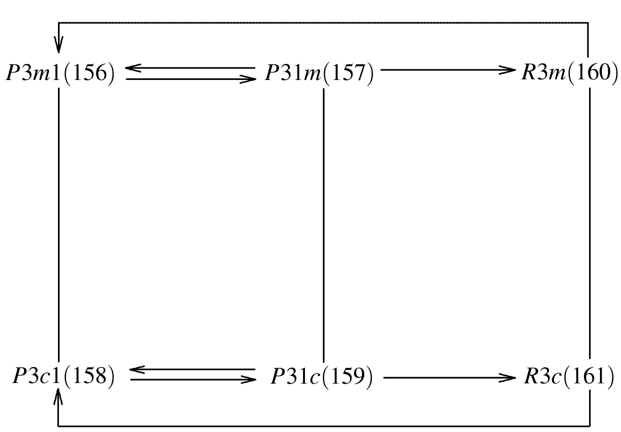

Fig. 2.5.3.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class $3m$.

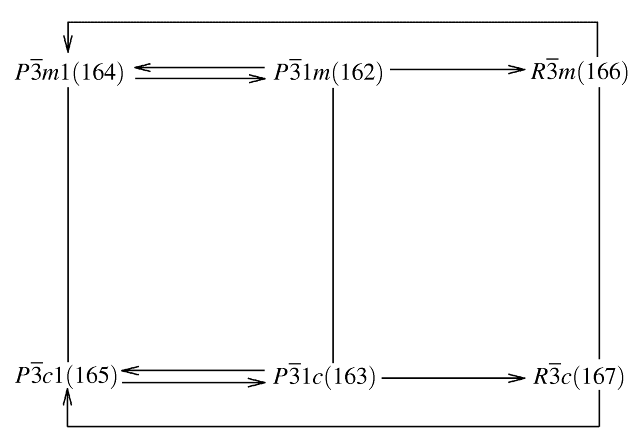

Fig. 2.5.3.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\overline{3}m$.

places, this may be more convenient, since no values for an origin shift have to be added. For this reason, the latter option is preferred in this case.

Origin shifts can be specified in terms of the coordinate system of the starting space group or of the coordinate system of the subgroup. In Part 2 of this volume, all origin shifts refer to the starting space group. In Part 3, the origin shifts are contained in the column 'Coordinates' as additive fractional numbers. This means that these shifts refer to the *coordinate system of the subgroup*.

When comparing related crystal structures, it is mainly the atomic coordinates which have to be interconverted. Thus the coordinate conversion formulae are needed anyway; they are given in the column 'Coordinates'. When space groups are involved that allow two origin choices, the origin shifts from a group to a subgroup can be different depending on whether origin choice 1 or 2 has been selected. Therefore, all space groups with two origin choices have two columns 'Coordinates', one for each origin choice. The coordinate conversion formulae for a specific subgroup in the two columns only differ in the additive fractional numbers that specify the origin shift. In addition, origin shifts could also have been specified in terms of the coordinate system of the starting space group. This, however, would have been redundant information that would have required an additional column, causing a serious shortage of space.

The origin shifts listed in the column 'Coordinates' can be converted to origin shifts that refer to the coordinate system of the starting space group in the following way:

Take:

$\mathbf{a}, \mathbf{b}, \mathbf{c}$	basis vectors of the starting space group;
O	origin of the starting space group;
$\mathbf{a}', \mathbf{b}', \mathbf{c}'$	basis vectors of the subgroup;
O'	origin of the subgroup;
$x_{o'}, y_{o'}, z_{o'}$	coordinates of O' expressed in the coordinate system of the starting group;
x'_o, y'_o, z'_o	coordinates of O expressed in the coordinate system of the subgroup.

The basis vectors are related according to

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

$\boldsymbol{P}$ is the 3×3 transformation matrix of the basis change. The origin shift $O \to O'$ then corresponds to the vector

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\boldsymbol{P} \begin{pmatrix} x'_o \\ y'_o \\ z'_o \end{pmatrix}.$$

Example 3.1.3.1.

In the group–subgroup relation $Fddd \to C12/c1$, a cell transformation and an origin shift are needed if origin choice 1 has been selected for $Fddd$. In the table for space group $Fddd$, No. 70, the transformation of the basis vectors in the column 'Axes' is given as $\mathbf{a}, -\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{c})$, which means that the transformation matrix is

$$\boldsymbol{P} = \begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}.$$

In the column 'Coordinates' for origin choice 1, the coordinate transformations are given as $x{-}z, -y+\frac{1}{8}, -2z+\frac{1}{4}$, which implies a coordinate shift of $x'_o = 0$, $y'_o = \frac{1}{8}$ and $z'_o = \frac{1}{4}$ referred to the coordinate system of the subgroup $C12/c1$, No. 15. The origin shift in terms of the starting space group $Fddd$ is

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{8} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{8} \\ \frac{1}{8} \\ \frac{1}{8} \end{pmatrix}.$$

Example 3.1.3.2.

Consider space group *Pnma*, No. 62, and its subgroup $P2_12_12_1$, No. 19. In the table for space group *Pnma*, the coordinate transformation in the column 'Coordinates' is given as $x, y, z+\frac{1}{4}$. Therefore, there is no basis transformation, $\boldsymbol{P} = \boldsymbol{I}$, but there is an origin shift of $x'_o = 0$, $y'_o = 0$, $z'_o = \frac{1}{4}$ expressed in the coordinate system of $P2_12_12_1$. In terms of the coordinate system of *Pnma* this coordinate shift has the opposite sign:

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}.$$

Note: In Chapter 2.3, the listed origin shifts refer to the starting space group and thus are given in a different way to that in Chapter 3.2. In addition, for a given group–subgroup pair the direction of the origin shift selected in Chapter 2.3 usually differs from the origin shift listed in Chapter 3.2 (often the direction is opposite; see the Appendix).

3.1.4. Nonconventional settings of orthorhombic space groups

Orthorhombic space groups can have as many as six different settings, as listed in Chapter 4.3 of Volume A. They result from the interchange of the axes **a**, **b**, **c** in the following ways:

Cyclic exchange: **b c a** or **c a b**.

Exchange of two axes, combined with the reversal of the direction of one axis in order to keep a right-handed coordinate system:

$\mathbf{b\,a\,\bar{c}}$ or $\mathbf{b\,\bar{a}\,c}$ or $\mathbf{\bar{b}\,a\,c}$;
$\mathbf{c\,b\,\bar{a}}$ or $\mathbf{c\,\bar{b}\,a}$ or $\mathbf{\bar{c}\,b\,a}$;
$\mathbf{a\,c\,\bar{b}}$ or $\mathbf{a\,\bar{c}\,b}$ or $\mathbf{\bar{a}\,c\,b}$.

The exchange has two consequences for a Hermann–Mauguin symbol:

(1) the symmetry operations given in the symbol interchange their positions in the symbol;
(2) the labels of the glide directions and of the centrings are interchanged.

In the same way, the sequences and the labels and values of the coordinate triplets have to be interchanged.

Example 3.1.4.1.

Take space group *Pbcm*, No. 57 (full symbol $P2/b2_1/c2_1/m$), and its Wyckoff position 4*c* $(x, \frac{1}{4}, 0)$. The positions in the symbol change as given by the arrows, and simultaneously the labels change:

abc: $P2/b2_1/c2_1/m$	$x, \frac{1}{4}, 0$	**abc**: $P2/b2_1/c2_1/m$	$x, \frac{1}{4}, 0$
bca: $P2_1/b2_1/m2/a$	$\frac{1}{4}, 0, z$	$\mathbf{b\bar{a}c}$: $P2_1/c\,2/a\,2_1/m$	$\frac{1}{4}, -y, 0$

The notation **b c a** means: the former *b* axis is now in the position of the *a* axis *etc.* or: convert *b* to *a*, *c* to *b*, and *a* to *c*.

	Axes	Coordinates	Wyckoff positions 2a	4b		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups										
[2] $P1$ (1)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x, 2y, y+z$;	$1a$	$2\times1a$	$P1$	$\frac{1}{2}(\mathbf{a}-\mathbf{c})$, $\mathbf{b}, \mathbf{c}$	$2x, y, y+z$	$P1$	$\mathbf{a}, \mathbf{b}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+z, y+z, 2z$
II Maximal *klassengleiche* subgroups										
Loss of centring translations										
[2] $P11b$ (7)		$x, y, z+\frac{1}{4}$	$2a$	$2\times2a$	$P11a$		$x, y, z+\frac{1}{4}$	$P11n$		$x, y, z+\frac{1}{4}$
[2] $P11m$ (6)			$1a; 1b$	$2\times2c$	$P11m$			$P11m$		
Enlarged unit cell, non-isomorphic										
[2] $A11a$ (9)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$4a$	$2\times4a$	$B11n$	$\mathbf{a}$, $\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11b$	$\mathbf{a}-\mathbf{b}$, $2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z$; $+(0, \frac{1}{2}, 0)$
[2] $A11a$ (9) $\widehat{=}\, I11b$	$2\mathbf{a}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$; $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+y, y, z$; $+(\frac{1}{2}, 0, 0)$; $x, \frac{1}{2}y, z+\frac{1}{4}$; $+(\frac{1}{2}, 0, 0)$	$4a$	$2\times4a$	$I11b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11b$	$\mathbf{a}+\mathbf{b}$, $2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-z+y), z$; $+(0, \frac{1}{2}, 0)$
Enlarged unit cell, isomorphic										
[3] $A11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$2a; 4b$	$3\times4b$	$B11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$I11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[p] $A11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$2a; \frac{p-1}{2}\times4b$	$p\times4b$	$B11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$I11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$
$p =$ prime > 2; $u = 1, \ldots, p-1$					$p =$ prime > 2; $u = 1, \ldots, p-1$			$p =$ prime > 2; $u = 1, \ldots, p-1$		
[2] $A11m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times2a$	$2\times4b$	$B11m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11m$	$\mathbf{a}-\mathbf{b}$, $2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z$; $+(0, \frac{1}{2}, 0)$
[2] $I11m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times2a$	$2\times4b$	$I11m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11m$	$\mathbf{a}+\mathbf{b}$, $2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-x+y), z$; $+(0, \frac{1}{2}, 0)$
[3] $A11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}$, $\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x-y), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $A11m$	$\mathbf{a}-\mathbf{b}$, $3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$\mathbf{a}+2\mathbf{b}$, $3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-2x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[3] $A11m$	$\mathbf{a}+\mathbf{b}$, $3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[3] $A11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times2a$	$3\times4b$	$B11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $+(0, \frac{1}{3}, 0)$	$I11m$	$\mathbf{a}-2\mathbf{b}$, $3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(2x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[p] $A11m$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$	$p\times2a$	$p\times4b$	$B11m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$I11m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $\pm(0, \frac{u}{p}, 0)$
$p =$ prime; $u = 1, \ldots, p-1$					$p =$ prime; $u = 1, \ldots, p-1$			$p =$ prime; > 2; $u = 1, \ldots, p-1$		
[p] $A11m$	$\mathbf{a}+q\mathbf{b}$, $p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z$; $+(0, \frac{u}{p}, 0)$	$p\times2a$	$p\times4b$	$B11m$	$p\mathbf{a}$, $q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-qy), y, z$; $+(\frac{u}{p}, 0, 0)$	$I11m$	$p\mathbf{a}$, $2q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-2qy), y, z$; $+(\frac{u}{p}, 0, 0)$
$p =$ prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$					$p =$ prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$p =$ prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$		

D_{2h}^{26} $I2/b2/a2/m$ No. 72 $Ibam$

	Axes	Coordinates	Wyckoff positions $4a$	$4b$	$4c$	$4d$	$8e$	$8f$	$8g$	$8h$	$8i$	$8j$	$16k$
I Maximal *translationengleiche* subgroups													
[2] $I2cm$ (46)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$8c$	$2\times4a$	$8c$	$8c$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}$ $Ima2$	**c**, −**b**, **a**	$z+\frac{1}{4},-y,x$											
[2] $Ic2m$ (46)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$8c$	$8c$	$2\times4a$	$8c$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}$ $Ima2$	**c**, **a**, **b**	$z+\frac{1}{4},x,y$											
[2] $Iba2$ (45)			$4a$	$4b$	$4a$	$4b$	$8c$	$8c$	$8c$	$2\times4a$	$2\times4b$	$8c$	$2\times8c$
[2] $I222$ (23)		$x,y,z+\frac{1}{4}$	$2a;2c$	$2b;2d$	$4i$	$4j$	$8k$	$4e;4f$	$4g;4h$	$2\times4i$	$2\times4j$	$8k$	$2\times8k$
[2] $I2/c11$ (15)			$4e$	$4e$	$4a$	$4b$	$4c;4d$	$2\times4e$	$8f$	$8f$	$8f$	$8f$	$2\times8f$
$\widehat{=}$ $I12/a1$	**c**, **a**, **b**	z,x,y											
$\widehat{=}$ $C12/c1$	−**b**−**c**, **a**, **c**	$-y,x,-y+z$											
[2] $I12/c1$ (15)			$4e$	$4e$	$4a$	$4b$	$4c;4d$	$8f$	$2\times4e$	$8f$	$8f$	$8f$	$2\times8f$
$\widehat{=}$ $C12/c1$	**a**−**c**, **b**, **c**	$x,y,x+z$											
[2] $I112/m$ (12)			$4g$	$4h$	$2a;2b$	$2c;2d$	$4e;4f$	$8j$	$8j$	$2\times4g$	$2\times4h$	$2\times4i$	$2\times8j$
$\widehat{=}$ $A112/m$	**b**, −**a**−**b**, **c**	$-x+y,-y,z$											
II Maximal *klassengleiche* subgroups													
Loss of centring translations													
[2] $Pbcn$ (60)			$4c$	$4c$	$4a$	$4b$	$8d$	$8d$	$2\times4c$	$8d$	$8d$	$8d$	$2\times8d$
[2] $Pcan$ (60)			$4c$	$4c$	$4a$	$4b$	$8d$	$2\times4c$	$8d$	$8d$	$8d$	$8d$	$2\times8d$
$\widehat{=}$ $Pbcn$	**b**, −**a**, **c**	$y,-x,z$											
[2] $Pbcm$ (57)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4d$	$4d$	$4a;4b$	$2\times4c$	$8e$	$8e$	$8e$	$2\times4d$	$2\times8e$
[2] $Pcam$ (57)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4d$	$4d$	$4a;4b$	$8e$	$2\times4c$	$8e$	$8e$	$2\times4d$	$2\times8e$
$\widehat{=}$ $Pbcm$	**b**, −**a**, **c**	$y+\frac{1}{4},-x-\frac{1}{4},z+\frac{1}{4}$											
[2] $Pccn$ (56)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4d$	$4c$	$4d$	$4a;4b$	$8e$	$8e$	$2\times4c$	$2\times4d$	$8e$	$2\times8e$
[2] $Pbam$ (55)			$4e$	$4f$	$2a;2b$	$2c;2d$	$8i$	$8i$	$8i$	$2\times4e$	$2\times4f$	$4g;4h$	$2\times8i$
[2] $Pban$ (50)	origin 1:	$x,y,z+\frac{1}{4}$	$2a;2d$	$2b;2c$	$4k$	$4l$	$4e;4f$	$4g;4h$	$4i;4j$	$2\times4k$	$2\times4l$	$8m$	$2\times8m$
	origin 2:	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$											
[2] $Pccm$ (49)			$2e;2h$	$2f;2g$	$2a;2b$	$2c;2d$	$8r$	$4i;4j$	$4k;4l$	$4m;4n$	$4o;4p$	$2\times4q$	$2\times8r$
Enlarged unit cell, isomorphic													
[3] $Ibam$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4c;8j$	$4d;8j$	$8e;16k$	$3\times8f$	$8g;16k$	$8h;16k$	$8i;16k$	$3\times8j$	$3\times16k$
[p] $Ibam$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$	$4a$; $\frac{p-1}{2}\times8f$	$4b$; $\frac{p-1}{2}\times8f$	$4c$; $\frac{p-1}{2}\times8j$	$4d$; $\frac{p-1}{2}\times8j$	$8e$; $\frac{p-1}{2}\times16k$	$p\times8f$	$8g$; $\frac{p-1}{2}\times16k$	$8h$; $\frac{p-1}{2}\times16k$	$8i$; $\frac{p-1}{2}\times16k$	$p\times8j$	$p\times16k$
	p = prime > 2; $u=1,\ldots,p-1$												
[3] $Ibam$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$4a;8g$	$4b;8g$	$4c;8j$	$4d;8j$	$8e;16k$	$8f;16k$	$3\times8g$	$8h;16k$	$8i;16k$	$3\times8j$	$3\times16k$
[p] $Ibam$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$	$4a$; $\frac{p-1}{2}\times8g$	$4b$; $\frac{p-1}{2}\times8g$	$4c$; $\frac{p-1}{2}\times8j$	$4d$; $\frac{p-1}{2}\times8j$	$8e$; $\frac{p-1}{2}\times16k$	$8f$; $\frac{p-1}{2}\times16k$	$p\times8g$	$8h$; $\frac{p-1}{2}\times16k$	$8i$; $\frac{p-1}{2}\times16k$	$p\times8j$	$p\times16k$
	p = prime > 2; $u=1,\ldots,p-1$												
[3] $Ibam$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$4a;8h$	$4b;8i$	$4c;8h$	$4d;8i$	$8e;16k$	$8f;16k$	$8g;16k$	$3\times8h$	$3\times8i$	$8j;16k$	$3\times16k$
[p] $Ibam$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$4a$; $\frac{p-1}{2}\times8h$	$4b$; $\frac{p-1}{2}\times8i$	$4c$; $\frac{p-1}{2}\times8h$	$4d$; $\frac{p-1}{2}\times8i$	$8e$; $\frac{p-1}{2}\times16k$	$8f$; $\frac{p-1}{2}\times16k$	$8g$; $\frac{p-1}{2}\times16k$	$p\times8h$	$p\times8i$	$8j$; $\frac{p-1}{2}\times16k$	$p\times16k$
	p = prime > 2; $u=1,\ldots,p-1$												

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Imcb$ $C\to A\to B$ $a\to b\to c\to a$ $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ $x\to y\to z\to x$

$Icma$ $A\to C\to B$ $a\leftarrow b\leftarrow c\leftarrow a$ $\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$ $x\leftarrow y\leftarrow z\leftarrow x$

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$1c$	$1d$	$2e$	$2f$	$2g$	$4h$
I Maximal *translationengleiche* subgroups										
[2] $P112\,(3)$			$1a$	$1a$	$1d$	$1d$	$2\times1a$	$2\times1d$	$1b;1c$	$2\times2e$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $I\bar{4}$ (82)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$4f$	$2c;2d$	$2\times4e$	$2\times4f$	$8g$	$2\times8g$
[2] $I\bar{4}$ (82)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$2c;2d$	$4f$	$2\times4e$	$2\times4f$	$8g$	$2\times8g$
Enlarged unit cell, isomorphic										
[2] $P\bar{4}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1b$	$2e$	$1c;1d$	$2f$	$2\times2e$	$2\times2f$	$2\times2g$	$2\times4h$
[2] $P\bar{4}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$	$1a;1b$	$2f$	$1c;1d$	$2\times2e$	$2\times2f$	$2\times2g$	$2\times4h$
[3] $P\bar{4}$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2e$	$1b;2e$	$1c;2f$	$1d;2f$	$3\times2e$	$3\times2f$	$3\times2g$	$3\times4h$
[p] $P\bar{4}$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$; $p=$ prime >2; $u=1,\ldots,p-1$	$1a;\frac{p-1}{2}\times2e$	$1b;\frac{p-1}{2}\times2e$	$1c;\frac{p-1}{2}\times2f$	$1d;\frac{p-1}{2}\times2f$	$p\times2e$	$p\times2f$	$p\times2g$	$p\times4h$
[2] $P\bar{4}$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a;1c$	$1b;1d$	$2g$	$2g$	$2e;2f$	$2\times2g$	$4h$	$2\times4h$
[2] $P\bar{4}$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2g$	$2g$	$1a;1c$	$1b;1d$	$2\times2g$	$2e;2f$	$4h$	$2\times4h$
[5] $P\bar{4}$	$\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z$; $\pm(\frac{1}{5},\frac{3}{5},0)$; $\pm(\frac{2}{5},\frac{1}{5},0)$	$1a;4h$	$1b;4h$	$1c;4h$	$1d;4h$	$2e;2\times4h$	$2f;2\times4h$	$2g;2\times4h$	$5\times4h$
[5] $P\bar{4}$	$\mathbf{a}-2\mathbf{b}$, $2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z$; $\pm(\frac{1}{5},\frac{2}{5},0)$; $\pm(\frac{3}{5},\frac{1}{5},0)$	$1a;4h$	$1b;4h$	$1c;4h$	$1d;4h$	$2e;2\times4h$	$2f;2\times4h$	$2g;2\times4h$	$5\times4h$
[p] $P\bar{4}$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z$; $+(\frac{uq}{p},\frac{ur}{p},0)$; $p=q^2+r^2=$ prime $=4n+1$; $q=2n+1\geq1$; $r=\pm2n'\neq0$; $u=1,\ldots,p-1$	$1a;\frac{p-1}{4}\times4h$	$1b;\frac{p-1}{4}\times4h$	$1c;\frac{p-1}{4}\times4h$	$1d;\frac{p-1}{4}\times4h$	$2e$; $\frac{p-1}{2}\times4h$	$2f$; $\frac{p-1}{2}\times4h$	$2g$; $\frac{p-1}{2}\times4h$	$p\times4h$
[9] $P\bar{4}$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;2\times4h$	$1b;2\times4h$	$1c;2\times4h$	$1d;2\times4h$	$2e;4\times4h$	$2f;4\times4h$	$2g;4\times4h$	$9\times4h$
[p^2] $P\bar{4}$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$; $p=$ prime $=4n-1$; $u,v=1,\ldots,p-1$	$1a;\frac{p^2-1}{4}\times4h$	$1b;\frac{p^2-1}{4}\times4h$	$1c;\frac{p^2-1}{4}\times4h$	$1d;\frac{p^2-1}{4}\times4h$	$2e$; $\frac{p^2-1}{2}\times4h$	$2f$; $\frac{p^2-1}{2}\times4h$	$2g$; $\frac{p^2-1}{2}\times4h$	$p^2\times4h$

$P3m1$ No. 156 C_{3v}^{1}

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$1c$	$3d$	$6e$
I Maximal *translationengleiche* subgroups							
[2] $P3$ (143)			$1a$	$1b$	$1c$	$3d$	$2\times3d$
[3] $C1m1$ (8)	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$2a$	$2a$	$2a$	$2a; 4b$	$3\times4b$
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$					
conjugate:	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z$					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $P3c1$ (158)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$2c$	$6d$	$2\times6d$
[3] $P31m$ (157)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	$1a; 2b$	$3c$	$3c$	$3c; 6d$	$3\times6d$
[3] $P31m$ (157)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	$3c$	$1a; 2b$	$3c$	$3c; 6d$	$3\times6d$
[3] $P31m$ (157)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	$3c$	$3c$	$1a; 2b$	$3c; 6d$	$3\times6d$
Enlarged unit cell, isomorphic							
[2] $P3m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times1a$	$2\times1b$	$2\times1c$	$2\times3d$	$2\times6e$
[3] $P3m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times1a$	$3\times1b$	$3\times1c$	$3\times3d$	$3\times6e$
[p] $P3m1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; $p=$ prime; $u=1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times1a$	$p\times1b$	$p\times1c$	$p\times3d$	$p\times6e$
[4] $P3m1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3d$	$1c; 3d$	$1b; 3d$	$2\times3d; 6e$	$4\times6e$
[p^2] $P3m1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; $p=$ prime $\neq 3$; $u,v=1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$1a; (p-1)\times3d$; $\frac{(p-1)(p-2)}{6}\times6e$	$1b(c^*)$; $(p-1)\times3d$; $\frac{(p-1)(p-2)}{6}\times6e$	$1c(b^*)$; $(p-1)\times3d$; $\frac{(p-1)(p-2)}{6}\times6e$	$p\times3d$; $\frac{p(p-1)}{2}\times6e$	$p^2\times6e$

* $p=3n-1$

$Pn\bar{3}n$ No. 222 $P4/n\,\bar{3}\,2/n$ O_h^2

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions $2a$	$6b$	$8c$	$12d$ $24g$	$12e$ $24h$	$16f$ $48i$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}3n$ (218)			$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$2a$	$6b$	$8e$	$6c; 6d$ $12g; 12h$	$12f$ $24i$	$2\times 8e$ $2\times 24i$
[2] $P432$ (207)			$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$1a; 1b$	$3c; 3d$	$8g$	$12h$ $2\times 12h$	$6e; 6f$ $12i; 12j$	$2\times 8g$ $2\times 24k$
[2] $Pn\bar{3}$ (201)				$2a$	$6d$	$4b; 4c$	$12g$ $2\times 12g$	$12f$ $24h$	$2\times 8e$ $2\times 24h$
[4] $R\bar{3}c$ (167)	(rhombohedral axes)	$x-\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$		$2a$	$6e$	$2b; 6d$	$12f$ $2\times 12f$	$12f$ $2\times 6e; 12f$	$4c; 12f$ $4\times 12f$
	a−**b**, **b**−**c**, **a**+**b**+**c** (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{4}$	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$6a$	$18e$	$6b; 18d$	$36f$ $2\times 36f$	$36f$ $2\times 18e; 36f$	$12c; 36f$ $4\times 36f$
conjugate:	−**a**−**b**, **b**+**c**, −**a**+**b**−**c** (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)-\frac{1}{4}$	$\frac{1}{3}(-2x-y+z)+\frac{1}{2}$, $\frac{1}{3}(-x+y+2z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-z)$						
conjugate:	**a**+**b**, −**b**+**c**, **a**−**b**−**c** (hex. axes)	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{4}$	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)+\frac{1}{2}$, $\frac{1}{3}(x-y-z)$						
conjugate:	−**a**+**b**, −**b**−**c**, −**a**−**b**+**c** (hex. axes)	$\frac{1}{3}(-2x+y-z)$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)-\frac{1}{4}$	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $P4/nnc$ (126)				$2a$	$2b; 4c$	$8f$	$4d; 8j$ $8g; 2\times 8j$	$4e; 8i$ $8h; 16k$	$16k$ $3\times 16k$
conjugate:	**b**, **c**, **a**	y, z, x	y, z, x						
conjugate:	**c**, **a**, **b**	z, x, y	z, x, y						

II Maximal *klassengleiche* subgroups
Enlarged unit cell, isomorphic

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$6b$	$8c$	$12d$ $24g$	$12e$ $24h$	$16f$ $48i$
[27] $Pn\bar{3}n$	3**a**, 3**b**, 3**c**	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$;	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$;	$2a; 12e; 16f; 24h$	$6b; 12e; 24g; 24h; 2\times 48i$	$8c; 16f; 4\times 48i$	$12d; 24g; 6\times 48i$ $3\times 24g; 12\times 48i$	$3\times 12e; 6\times 48i$ $3\times 24h; 12\times 48i$	$3\times 16f; 8\times 48i$ $27\times 48i$
		(both origins): $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$							
$[p^3]$ $Pn\bar{3}n$	p**a**, p**b**, p**c** p = prime > 2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a; \frac{p-1}{2}\times 12e$; $\frac{p-1}{2}\times 16f$ $\frac{p-1}{2}\times 24h$; $\frac{p^3-13p+12}{24}\times 48i$	$6b; \frac{p-1}{2}\times 12e$; $\frac{p-1}{2}\times 24g$; $\frac{p-1}{2}\times 24h$; $\frac{p^3-5p+4}{8}\times 48i$	$8c$; $\frac{p-1}{2}\times 16f$; $\frac{p(p^2-1)}{6}\times 48i$	$12d$; $\frac{p-1}{2}\times 24g$; $\frac{p(p^2-1)}{4}\times 48i$ $p\times 24g$; $\frac{p(p^2-1)}{2}\times 48i$	$p\times 12e$; $\frac{p(p^2-1)}{4}\times 48i$ $p\times 24h$; $\frac{p(p^2-1)}{2}\times 48i$	$p\times 16f$; $\frac{p(p^2-1)}{3}\times 48i$ $p^3\times 48i$