# INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

Volume A1 SYMMETRY RELATIONS BETWEEN SPACE GROUPS

> *Edited by* H. WONDRATSCHEK AND U. MÜLLER

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# 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 *Inter-*



national Tables for Crystallography Volume A (1983). The tables in his book Geometrische Kristallographie des Diskontinuums (1919) contained the 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 (1898–1961) 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, and Professor M. I. Aroyo 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. We thank Professor H. Bärnighausen, Universität Karlsruhe, Germany, for discussions and advice on Chapter 1.6.

In the late 1960s and early 1970s, J. Neubüser and his team at RWTH Aachen 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.

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, around 1970. M. I. Aroyo 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, 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.

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# Contents

# PAGE

Foreword (Th. Hahn)	ix
Scope of this volume (M. I. Aroyo, U. Müller and H. Wondratschek)	x
Computer production of Parts 2 and 3 (P. Konstantinov, A. Kirov, E. B. Kroumova, M. I. Aroyo and U. Müller)	xi
List of symbols and abbreviations used in this volume	xii

# PART 1. SPACE GROUPS AND THEIR SUBGROUPS

1.1. Historical introduction (M. I. Aroyo, U. Müller and H. Wondratschek)		 	 	 	 	••	 ••	 	2
1.1.1. The fundamental laws of crystallography		 	 	 	 		 	 	2
1.1.2. Symmetry and crystal-structure determination		 	 	 	 		 	 	2
1.1.3. Development of the theory of group-subgroup relations		 	 	 	 		 	 	3
1.1.4. Applications of group-subgroup relations		 	 	 	 		 	 	4
<b>1.2. General introduction to the subgroups of space groups</b> (H. WONDRATSCHEK)		 	 	 	 		 	 	7
1.2.1. General remarks		 	 	 	 		 	 	7
1.2.2. Mappings and matrices		 	 	 	 		 	 	7
<b>1.2.3.</b> Groups		 	 	 	 		 	 	10
<b>1.2.4.</b> Subgroups		 	 	 	 		 	 	12
<b>1.2.5.</b> Space groups		 	 	 	 		 ••	 	14
<b>1.2.6.</b> Types of subgroups of space groups		 	 	 	 		 ••	 	18
1.2.7. Application to domain structures		 	 	 	 		 	 	20
1.2.8. Lemmata on subgroups of space groups		 	 	 	 		 	 	23
1.3. Computer checking of the subgroup data (F. Gähler)		 	 	 	 		 	 	25
1.3.1. Introduction		 	 	 	 		 	 	25
<b>1.3.2.</b> Basic capabilities of the <i>Cryst</i> package		 	 	 	 		 	 	25
<b>1.3.3.</b> Computing maximal subgroups		 	 	 	 		 	 	25
<b>1.3.4.</b> Description of the checks		 	 	 	 		 	 	26
1.4. The mathematical background of the subgroup tables (G. NEBE)		 	 	 	 		 	 	27
1.4.1. Introduction		 	 	 	 		 	 	27
<b>1.4.2.</b> The affine space		 	 	 	 		 	 	27
1.4.3. Groups		 	 	 	 		 	 	29
<b>1.4.4.</b> Space groups		 	 	 	 		 	 	33
1.4.5. Maximal subgroups		 	 	 	 		 	 	35
<b>1.4.6. Quantitative results</b>		 	 	 	 		 	 	37
1.4.7. Qualitative results		 	 	 	 		 	 	38
<b>1.4.8. Minimal supergroups</b>		 	 	 	 		 	 	39
1.5. Remarks on Wyckoff positions (U. MÜLLER)		 	 	 	 		 	 	41
1.5.1. Crystallographic orbits and Wyckoff positions		 	 	 	 		 	 	41
1.5.2. Derivative structures and phase transitions		 	 	 	 		 	 	41
1.5.3. Relations between the positions in group-subgroup relations		 	 	 	 		 	 	42
1.6. Relating crystal structures by group-subgroup relations (U. Müller)		 	 	 	 		 	 	44
1.6.1. Introduction		 	 	 	 		 	 	44
1.6.2. The symmetry principle in crystal chemistry		 	 	 	 		 	 	44
1.6.3. Bärnighausen trees		 	 	 	 		 	 	44
1.6.4. The different kinds of symmetry relations among related crystal structu	ires	 	 	 	 		 	 	46

# CONTENTS

1.6.6. Comments concerning phase transitions and twin domains	54
<b>1.6.7.</b> Exercising care in the use of group-subgroup relations	54
1.7. The Bilbao Crystallographic Server (M. I. AROYO, J. M. PEREZ-MATO, C. CAPILLAS AND H. WONDRATSCHEK)	57
	57
1.7.2. Databases and retrieval tools	57
1.7.3. Group-subgroup and group-supergroup relations between space groups	58
1.7.4. Relations of Wyckoff positions for a group-subgroup pair of space groups	66
PART 2. MAXIMAL SUBGROUPS OF THE PLANE GROUPS AND SPACE GROUPS	
2.1. Guide to the subgroup tables and graphs (H. Wondratschek and M. I. Aroyo)	72
2.1.1. Contents and arrangement of the subgroup tables	72
2.1.2. Structure of the subgroup tables	72
2.1.3. I Maximal translationengleiche subgroups (t-subgroups)	76
2.1.4. II Maximal <i>klassengleiche</i> subgroups ( <i>k</i> -subgroups)	79
<b>2.1.5. Series of maximal isomorphic subgroups</b> (Y. BILLIET)	82
2.1.6. The data for minimal supergroups	84
2.1.7. Derivation of the minimal supergroups from the subgroup tables	86
<b>2.1.8.</b> The subgroup graphs	90
2.2. Tables of maximal subgroups of the plane groups (Y. Billiet, M. I. Aroyo and H. Wondratschek)	97
2.3. Tables of maximal subgroups of the space groups (Y. Billiet, M. I. Aroyo and H. Wondratschek)	115
2.4. Graphs for <i>translationengleiche</i> subgroups (V. GRAMLICH AND H. WONDRATSCHEK)	433
2.4.1. Graphs of the translationengleiche subgroups with a cubic summit	434
2.4.2. Graphs of the <i>translationengleiche</i> subgroups with a tetragonal summit	440
2.4.3. Graphs of the <i>translationengleiche</i> subgroups with a hexagonal summit	447
2.4.4. Graphs of the <i>translationengleiche</i> subgroups with an orthorhombic summit	450
2.5. Graphs for <i>klassengleiche</i> subgroups (V. GRAMLICH AND H. WONDRATSCHEK)	453
251 Graphs of the <i>klassengleiche</i> subgroups of monoclinic and orthorhombic space groups	454
2.5.1. Graphs of the <i>klassengleiche</i> subgroups of tetragonal space groups	457
2.5.2. Graphs of the <i>klassengleiche</i> subgroups of trigonal space groups	460
2.5.5. Graphs of the <i>klassengleiche</i> subgroups of heyagonal space groups	461
2.5.4. Graphs of the <i>klassengleiche</i> subgroups of rubic space groups	462
	402
PART 3. RELATIONS BETWEEN THE WYCKOFF POSITIONS	
<b>3.1.</b> Guide to the tables (U. Müller)	466
3.1.1. Arrangement of the entries	466
3.1.2. Cell transformations	468
3.1.3. Origin shifts	468
3.1.4. Nonconventional settings of orthorhombic space groups	469
3.1.5. Conjugate subgroups	470
3.1.6. Monoclinic and triclinic subgroups	471
3.2. Tables of the relations of the Wyckoff positions (U. Müller)	473
Appendix. Differences in the presentation of Parts 2 and 3 (U. Müller and H. Wondratschek)	761
Subject index	763

# By Th. 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, Section 2.2.15): *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.

In the second edition of Volume A1 (2010), additional aspects of group–subgroup relations are included; in particular procedures for the derivation of the minimal supergroups of the space groups are described. Now the minimal supergroups can be calculated from the data for the maximal subgroups to the full extent, with the exception of the low-symmetry (triclinic and monoclinic) space groups. Two new chapters on trees of group– subgroup relations (Bärnighausen trees) and on the Bilbao Crystallographic Server bring these tools closer to the user.

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 primary subject of this volume, are an important tool in crystallographic, physical and chemical investigations of solids. These relations are complemented by the corresponding relations between the Wyckoff positions of the group-subgroup pairs.

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, among them to the 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, on group–subgroup relations and on the underlying mathematical background, this volume provides the reader 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 their 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 the nonisomorphic subgroups.
- (4) The listings of Volume A for the non-isomorphic supergroups for all 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 all the Wyckoff positions for each space group with their splittings and/or site-symmetry reductions if the symmetry is reduced to that of a maximal subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained directly from the coordinates in the original space group.

In this second edition all misprints and errors found up to now have been corrected and the number of illustrating examples has been increased.

In addition, a few changes and extensions have been introduced to facilitate the use of the volume and to extend its range:

- (7) The subgroup tables, in particular those of the isomorphic subgroups, have been homogenized.
- (8) The data for the minimal supergroups are sufficient to derive all minimal supergroups starting from the subgroup data, with the exception of the *translationengleiche* supergroups of triclinic and monoclinic space groups. The procedures by which this derivation can be achieved are described in detail. The supergroup data are useful for the prediction of hightemperature 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.
- (9) A new chapter is devoted to the construction of family trees connecting crystal structures (Bärnighausen trees). In a Bärnighausen tree the relations between the Wyckoff positions occupied in the different crystal structures are accompanied by the relations between the corresponding group-subgroup pairs of space groups. Such trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases:
  - (*a*) the possibility of distortions due to reduction of site symmetries;
  - (b) chemical variations (atomic substitutions) allowed for atomic positions that have become symmetryindependent.

Bärnighausen trees visualize in a compact manner the structural relations between different polymorphic modifications involved in a phase transition and enable the comparison of crystal structures and their classification into crystal-structure types.

(10) A new chapter is dedicated to the Bilbao Crystallographic Server, http://www.cryst.ehu.es/. The server offers freely accessible crystallographic databases and computer programs, in particular those related to the contents of this volume. The available computer tools permit the studies of general group-subgroup relations between space groups and the corresponding Wyckoff positions.

The 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 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.

# **Computer production of Parts 2 and 3**

BY PRESLAV KONSTANTINOV, ASEN KIROV, ELI B. KROUMOVA, MOIS I. AROYO AND ULRICH MÜLLER

The tables of this volume were produced electronically using the LATEX  $2_{\varepsilon}$  typesetting system [Lamport (1994). A Document Preparation System. 2nd ed. Reading: Addison-Wesley], which has the following advantages:

- (1) correcting and modifying the layout and the data are easy;
- (2) correcting or updating these for further editions of this volume should also be simple;
- (3) the cost of production for the first edition and later editions should be kept low.

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  $2_{\varepsilon}$  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  $2_{\varepsilon}$  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 or pdf 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  $LATEX 2_{\varepsilon}$  files were either keyed by hand or computer-generated. The preparation of the data files of Part 2 can be summarized as follows:

- (i) Headline, origin: hand-keyed.
- (ii) Generators: hand-keyed.
- (iii) 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.
- (iv) 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.
- (v) Minimal supergroups: created automatically from the data for maximal subgroups.

The electronic preparation of the subgroup tables 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 1.3) 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). *POWDER CELL. Computer program for the calculation of X-ray powder diagrams.* Bundesanstalt für Materialforschung, Berlin]. In addition, all relations were cross-checked with the program *WYCKSPLIT* [Kroumova *et al.* (1998). *J. Appl. Cryst.* **31**, 646; http://www. cryst.ehu.es/cryst/wpsplit.html], 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	(4) (	Groups	
P, Q, R, X	points	${\mathcal G}$		group; space group
0	origin	${\mathcal R}$		space group (Chapter 1.4)
$A_n, \mathbb{A}_n, P_n$	<i>n</i> -dimensional affine space	$\mathcal{H},\mathcal{U}$	l	subgroups of $\mathcal{G}$
$E_n, \mathbb{E}_n$	<i>n</i> -dimensional Euclidean point space	$\mathcal{M}$		maximal subgroup of $\mathcal{G}$ (Chapter 1.4)
$x, y, z$ ; or $x_i$	point coordinates	$\mathcal{M}$		Hermann's group (Chapters 1.2, 1.7, 2.1)
x	column of point coordinates	$\mathcal{P},\mathcal{S}$	$\mathcal{V},\mathcal{V},\mathcal{Z}$	groups or sets of group elements, e.g. cosets
$\tilde{X}$	image point	$\mathcal{T}(\mathcal{G})$	), $\mathcal{T}(\mathcal{R})$	group of all translations of $\mathcal{G}, \mathcal{R}$
ĩ	column of coordinates of an image point	nt $\mathcal{A}$		group of all affine mappings = affine group
$\tilde{x}_i$	coordinates of an image point	ε		group of all isometries (motions)
<i>x</i> ′	column of coordinates in a new coordin	nate		= Euclidean group
	system (after basis transformation)	${\cal F}$		factor group
$x'_i$	coordinates in a new coordinate system	ı I		trivial group, consisting of the unit element <i>e</i> only
		$\mathcal{N}$		normal subgroup
		$\mathcal{O}$		group of all orthogonal mappings = orthogonal group
(2) Vectors and	l vector space	$\mathcal{N}_{\mathcal{G}}(\mathcal{I})$	H)	normalizer of $\mathcal{H}$ in $\mathcal{G}$
<b>a</b> , <b>b</b> , <b>c</b> ; or <b>a</b> <sub>i</sub>	basis vectors of the space	$\mathcal{N}_{\mathcal{E}}(\mathcal{I})$	H)	Euclidean normalizer of $\mathcal{H}$
r, x	vectors, position vectors	$\mathcal{N}_{\mathcal{A}}(\mathbf{C})$	H)	affine normalizer of $\mathcal{H}$
0	zero vector (all coefficients zero)	$\mathcal{P}_{\mathcal{G}}, \mathcal{T}$	$\mathcal{P}_{\mathcal{H}}$	point groups of the space groups $\mathcal{G}, \mathcal{H}$
a, b, c	lengths of basis vectors latti	ce $\mathcal{S}_{\mathcal{G}}(\lambda)$	$\mathcal{S}_{\mathcal{H}}(X)$	site-symmetry groups of point $X$ in the space
$\alpha, \beta, \gamma$ ; or $\alpha_j$	angles between basis vectors f para	imeters		groups $\mathcal{G}, \mathcal{H}$
r	column of vector coefficients	a, b,	g, h, m, t	group elements
r <sub>i</sub>	vector coefficients	е		unit element
$(\mathbf{a})^{\mathrm{T}}$	row of basis vectors	$2, 2_1$	, <b>m</b> , <b>1</b> ,	symmetry operations
$\mathbf{V}_n$	<i>n</i> -dimensional vector space	<i>i</i> or	[ <i>i</i> ]	index of $\mathcal{H}$ in $\mathcal{G}$

# (5) Symbols used in the tables*n* prime number > 1

		p	prime number > 1
(3) Mappings and their matrices and columns		n, n', n'', n'''	arbitrary positive integer numbers
A, W	$(3 \times 3)$ matrices	q, r, u, v, w	arbitrary integer numbers in the given range
$A^{\mathrm{T}}$	matrix A transposed	a, b, c	basis vectors of the space group
Ι	$(3 \times 3)$ unit matrix	a', b', c'	basis vectors of the subgroup or supergroup
$A_{ik}, W_{ik}$	coefficients	<i>x</i> , <i>y</i> , <i>z</i>	point coordinates in the space group
(A, a), (W, w)	matrix-column pairs	t(1, 0, 0),	generating translations
W	augmented matrix	$t(0, 1, 0), \ldots$	
x, x̃, t	augmented columns		
<b>P</b> , P	transformation matrices		
A, I, W	mappings	(6) Abbreviatio	ons
w	column of the translation part of a mapping	HM symbol	Hermann–Mauguin symbol
Wi	coefficients of the translation part of a	IT A	International Tables for Crystallography
	mapping		Volume A
$\boldsymbol{G},G_{ik}$	fundamental matrix and its coefficients	PCA	parent-clamping approximation

det( . . . )

tr( . . . )

determinant of a matrix

trace of a matrix

PCA	parent-clamping approximation
k-subgroup	klassengleiche subgroup

t-subgroup	translationengleiche subgroup
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# **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*.<sup>1</sup>

*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.  $\Box$

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 **t** and has no fixed point: if  $\mathbf{x}$  is the column of coordinates of a point P, then the coordinates  $\tilde{\mathbf{x}}$  of the image point  $\tilde{P}$  are  $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{t}$ . If a translation is a symmetry operation of an object, the object extends infinitely in the directions of **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  $\varphi$ . In particular, a rotation is called an *N*-fold rotation if the rotation angle is  $\varphi = k \times 360^{\circ}/N$ , 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

<sup>&</sup>lt;sup>1</sup> A real single crystal is still different from a macroscopic crystal. There are dislocations, point defects like vacancies, interstitial atoms or replacements of atoms, and the atoms are never at rest but vibrate. Therefore, the macroscopic crystal is a more-or-less strongly idealized model of the real crystal.

# 1.4. The mathematical background of the subgroup tables

### BY GABRIELE NEBE

### 1.4.1. 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 (threedimensional) 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 1.4.2, 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 *International Tables for Crystallography* Volume A (2005) (abbreviated as *IT* A) or the book by Hahn & Wondratschek (1994).

Section 1.4.3 gives an introduction to abstract groups and states the important theorems of group theory that will be applied in Section 1.4.4 to the most important groups in crystal-lography, the space groups. In particular, Section 1.4.4 treats maximal subgroups of space groups which have a special structure by the theorem of Hermann. In Section 1.4.5, 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 1.4.6. The next section, Section 1.4.7, deals with the very subtle question of when these maximal subgroups of a space group are isomorphic to this space group. In Section 1.4.8 minimal supergroups of space groups are treated briefly.

### 1.4.2. The affine space

# 1.4.2.1. 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 contains the positions of atoms in crystals (the so-called 'points'). 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, for example, 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 (for a description, see Opgenorth et al., 1998).

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 **o**. It is characterized by the property that  $\mathbf{v} + \mathbf{o} = \mathbf{v}$  for all vectors **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 higherdimensional vector space, where the addition of a point and a vector makes sense.

#### 1.4.2.2. 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

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

(In crystallography *n* is normally 3.) The entries  $x_1, \ldots, x_n$  are called the *coefficients* of the vector **x**. On **V**<sub>n</sub> 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

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

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

# 1.5. Remarks on Wyckoff positions

# By Ulrich Müller

#### 1.5.1. 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, 2005; 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,  $0, \frac{1}{2}, 0.391$  makes 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* (2005). They are labelled with letters  $a, b, \ldots$ , 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, 2005).

#### Example 1.5.1.1

In space group *I*222, 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 *I*222, which is isomorphic to  $Pm\bar{3}m$ , 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 *I*222.

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.*, 2005). In Example 1.5.1.1 (space group *I*222), the positions 4*e* and 4*f* are equivalent under the Euclidean normalizer (and so are 4*g*, 4*h* and also 4*i*, 4*j*). The Euclidean normalizer of the space group *I*222 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 4*e* and 4*f* as well as 4*g* and 4*h* of *I*222.

#### *Example 1.5.1.2*

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 1.5.1.3

In diamond, the carbon atoms occupy the orbit belonging to the Wyckoff position 8*a* of the space group  $Fd\overline{3}m$ , No. 227. Zinc blende (sphalerite) crystallizes in the maximal subgroup  $F\overline{4}3m$ , No. 216, of  $Fd\overline{3}m$ . With the transition  $Fd\overline{3}m \rightarrow F\overline{4}3m$ the Wyckoff position 8*a* splits into the positions 4*a* and 4*c* of  $F\overline{4}3m$ . These are two symmetry-independent positions that allow an occupation by atoms of two different elements (zinc and sulfur). In this example, all of the positions retain the site symmetry  $\overline{4}3m$  and each Wyckoff position comprises only one orbit.

#### 1.5.2. Derivative structures and phase transitions

In crystal chemistry, structural relations such as the relation diamond-sphalerite are of fundamental interest. Structures that result from a *basic structure* by the substitution of atoms of one kind for atoms of different elements, the topology being retained, are called *derivative structures* after Buerger (1947, 1951). For the basic structure the term *aristotype* has also been coined, while its derivative structures are called *hettotypes* (Megaw, 1973). For more details, see Chapter 1.6. When searching for derivative structures, one must look for space groups that are subgroups of the space group of the aristotype *and* in which the orbit of the atom(s) to be substituted splits into different orbits.

Similar relations also apply to many phase transitions (*cf.* Section 1.6.6). Very often the space group of one of the phases is a subgroup of the space group of the other. For second-order phase transitions this is even mandatory (*cf.* Section 1.2.7). The positions of the atoms in one phase are related to those in the other one.

### Example 1.5.2.1

The disorder–order transition of  $\beta$ -brass (CuZn) taking place at 741 K involves a space-group change from the space group

# **1.6. Relating crystal structures by group–subgroup relations**

# By Ulrich Müller

# 1.6.1. 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 (see following sections).
- (2) Elucidation of problems concerning twinned crystals and antiphase domains (see Section 1.6.6).
- (3) Changes of structures and physical properties taking place during phase transitions; applications of Landau theory (Aizu, 1970; Aroyo & Perez-Mato, 1998; Birman, 1966*a*,*b*, 1978; Cracknell, 1975; Howard & Stokes, 2005; Igartua *et al.*, 1996; Izyumov & Syromyatnikov, 1990; Landau & Lifshitz, 1980; Lyubarskii, 1960; Salje, 1990; Stokes & Hatch, 1988; Tolédano & Tolédano, 1987).
- (4) Prediction of crystal-structure types and calculation of the numbers of possible structure types (see Section 1.6.4.7).
- (5) Solution of the phase problem in the crystal structure analysis of proteins (Di Costanzo *et al.*, 2003).

Bärnighausen (1975, 1980) presented a standardized procedure to set forth structural relations between crystal structures with the aid of symmetry relations between their space groups. For a review on this subject see Müller (2004). Short descriptions are given by Chapuis (1992) and Müller (2006). The main concept is to start from a simple, highly symmetrical crystal structure and to derive more and more complicated structures by distortions and/or substitutions of atoms. Similar to the 'diagrams of lattices of subgroups' used in mathematics, a tree of group-subgroup relations between the space groups involved, now called a Bärnighausen tree, serves as the main guideline. The highly symmetrical starting structure is called the aristotype after Megaw (1973) or basic structure after Buerger (1947, 1951); other terms used in the literature on phase transitions in physics are prototype or parent structure. The derived structures are the hettotypes or derivative structures. In Megaw's (1973) terminology, the structures mentioned in the tree form a *family of structures*.

The structure type to be chosen as the aristotype depends on the specific problem and, therefore, the term aristotype cannot be defined in a strict manner. For example, a body-centred packing of spheres (space group  $Im\overline{3}m$ ) can be chosen as the aristotype for certain intermetallic structures. By symmetry reduction due to a loss of the centring, the CsCl type (space group  $Pm\overline{3}m$ ) can be derived. However, if all the structures considered are ionic, there is no point in starting from the body-centred packing of spheres and one can choose the CsCl type as the aristotype.

## 1.6.2. The symmetry principle in crystal chemistry

The usefulness of symmetry relations is intimately related to the symmetry principle in crystal chemistry. This is an old principle based on experience which has been worded during its long history in rather different ways. Bärnighausen (1980) summarized it in the following way:

- (1) In crystal structures the arrangement of atoms reveals a pronounced tendency towards the highest possible symmetry.
- (2) Counteracting factors due to special properties of the atoms or atom aggregates may prevent the attainment of the highest possible symmetry. However, in most cases the deviations from the ideal symmetry are only small (key word: pseudosymmetry).
- (3) During phase transitions and solid-state reactions which result in products of lower symmetry, the higher symmetry of the starting material is often indirectly preserved by the formation of oriented domains.

Aspect (1) is due to the tendency of atoms of the same kind to occupy equivalent positions, as stated by Brunner (1971). This has physical reasons: depending on chemical composition, the kind of chemical bonding, electron configuration of the atoms, relative sizes of the atoms, pressure, temperature *etc.*, there exists *one* energetically most favourable surrounding for atoms of a given species which all of these atoms strive to attain.

Aspect (2) of the symmetry principle is exploited in the following sections. Factors that counteract the attainment of the highest symmetry include: (1) stereochemically active lone electron pairs; (2) Jahn–Teller distortions; (3) covalent bonds; (4) Peierls distortions; (5) ordered occupation of originally equivalent sites by different atomic species (substitution derivatives); (6) partial occupation of voids in a packing of atoms; (7) partial vacation of atomic positions; (8) freezing (condensation) of lattice vibrations (soft modes) giving rise to phase transitions; and (9) ordering of atoms in a disordered structure.

Aspect (3) of the symmetry principle has its origin in an observation by Bernal (1938). He noted that in the solid state reaction  $Mn(OH)_2 \rightarrow MnOOH \rightarrow MnO_2$  the starting and the product crystal had the same orientation. Such reactions are called topotactic reactions after Lotgering (1959) (for a more exact definition see Giovanoli & Leuenberger, 1969). In a paper by Bernal & Mackay (1965) we find the sentence: 'One of the controlling factors of topotactic reactions is, of course, symmetry. This can be treated at various levels of sophistication, ranging from Lyubarskii's to ours, where we find that the simple concept of Buridan's ass illumines most cases.' According to the metaphor of Buridan (French philosopher, died circa 1358), the ass starves to death between two equal and equidistant bundles of hay because it cannot decide between them. Referred to crystals, such an asinine behaviour would correspond to an absence of phase transitions or solid-state reactions if there are two or more energetically equivalent orientations of the domains of the product. Crystals, of course, do not behave like the ass; they take both.

#### 1.6.3. Bärnighausen trees

To represent symmetry relations between different crystal structures in a concise manner, we construct a tree of group– subgroup relations in a modular design, beginning with the space group of the aristotype at its top. Each module represents one

# 1.7. The Bilbao Crystallographic Server

BY MOIS I. AROYO, J. MANUEL PEREZ-MATO, CESAR CAPILLAS AND HANS WONDRATSCHEK

#### 1.7.1. Introduction

The Bilbao Crystallographic Server, http://www.cryst.ehu.es, is a web site of crystallographic databases and programs. It can be used free of charge from any computer with a web browser *via* the Internet.

The server is built on a core of databases and contains different shells. The set of databases includes data from the 5th edition of *International Tables for Crystallography* Volume A, *Space-Group Symmetry* (2005) (hereafter referred to as *IT* A) and the data for maximal subgroups of space groups as listed in Part 2 of this volume (hereafter referred to as *IT* A1). Access is also provided to the crystallographic data for the subperiodic layer and rod groups [*International Tables for Crystallography*, Volume E, *Subperiodic Groups* (2002)] and their maximal subgroups. A database on incommensurate structures incorporating modulated structures and composites, and a **k**-vector database with Brillouin-zone figures and classification tables of the wavevectors for space groups are also available.

Communication with the databases is achieved by simple retrieval tools. They allow access to the information on space groups or subperiodic groups in different types of formats: HTML, text ASCII or XML. The next shell includes programs related to group–subgroup relations of space groups. These programs use the retrieval tools for accessing the necessary space-group information and apply group-theoretical algorithms in order to obtain specific results which are not available in the databases. There follows a shell with programs on representation theory of space groups and point groups and further useful symmetry information. Parallel to the crystallographic software, a shell with programs facilitating the study of specific problems related to solid-state physics, structural chemistry and crystallography has also been developed.

The server has been operating since 1998, and new programs and applications are being added (Kroumova, Perez-Mato, Aroyo *et al.*, 1998; Aroyo, Perez-Mato *et al.*, 2006; Aroyo, Kirov *et al.*, 2006). The aim of the present chapter is to report on the different databases and programs of the server related to the subject of this volume. Parts of these databases and programs have already been described in Aroyo, Perez-Mato *et al.* (2006), and here we follow closely that presentation. The chapter is completed by the description of the new developments up to 2007.

The relevant databases and retrieval tools that access the stored symmetry information are presented in Section 1.7.2. The discussion of the accompanying applications is focused on the crystallographic computing programs related to group-subgroup and group-supergroup relations between space groups (Section 1.7.3). The program for the analysis of the relations of the Wyckoff positions for a group-subgroup pair of space groups is presented in Section 1.7.4. The underlying group-theoretical background of the programs is briefly explained and details of the necessary input data and the output are given. The use of the programs is demonstrated by illustrative examples.

### 1.7.2. Databases and retrieval tools

The databases form the core of the Bilbao Crystallographic Server and the information stored in them is used by all computer programs available on the server. The following description is restricted to the databases related to the symmetry relations between space groups; these are the databases that include space-group data from *IT* A and subgroup data from *IT* A1.

#### 1.7.2.1. Space-group data

The programs and databases of the Bilbao Crystallographic Server use specific settings of space groups (hereafter referred to as *standard* or *default* settings) that coincide with the conventional space-group descriptions found in *IT* A. For space groups with more than one description in *IT* A, the following settings are chosen as standard: unique axis *b* setting, cell choice 1 for monoclinic groups; hexagonal axes setting for rhombohedral groups; and origin choice 2 (origin at  $\overline{1}$ ) for the centrosymmetric groups listed with respect to two origins in *IT* A.

The space-group database includes the following symmetry information:

- (i) The generators and the representatives of the general position of each space group specified by its *IT* A number and Hermann–Mauguin symbol;
- (ii) The special Wyckoff positions including the Wyckoff letter, Wyckoff multiplicity, the site-symmetry group and the set of coset representatives, as given in *IT* A;
- (iii) The reflection conditions including the general and special conditions;
- (iv) The affine and Euclidean normalizers of the space groups (cf. IT A, Part 15). They are described by sets of additional symmetry operations that generate the normalizers successively from the space groups. The database includes the additional generators of the Euclidean normalizers for the general-cell metrics as listed in Tables 15.2.1.3 and 15.2.1.4 of IT A. These Euclidean normalizers are also affine normalizers for all cubic, hexagonal, trigonal, tetragonal and part of the orthorhombic space-group types. For the rest of the orthorhombic space groups, the type of the affine normalizer coincides with the highest-symmetry Euclidean normalizer of that space group and the corresponding additional generators form part of the database (cf. Table 15.2.1.3 of IT A). The affine normalizers of triclinic and monoclinic groups are not isomorphic to groups of motions and they are not included in the normalizer database of the Bilbao Crystallographic Server.
- (v) The assignment of Wyckoff positions to Wyckoff sets as found in Table 14.2.3.2 of *IT* A.

The data from the databases can be accessed using the simple retrieval tools, which use as input the number of the space group (*IT* A numbers). It is also possible to select the group from a table of *IT* A numbers and Hermann–Mauguin symbols. The output of the program *GENPOS* contains a list of the generators or the general positions and provides the possibility to obtain the same data in different settings either by specifying the transformation

# 2.1. Guide to the subgroup tables and graphs

BY HANS WONDRATSCHEK AND MOIS I. AROYO; YVES BILLIET (SECTION 2.1.5)

#### 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. The subgroup data are listed either individually, or as members of (infinite) series, or both. The supergroup data are not as complete as the subgroup data. However, most of them can be obtained by proper evaluation of the subgroup data, as shown in Section 2.1.7. 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* (2005), 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 solid line 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. Graphs for *translationengleiche* and *klassengleiche* subgroups are found in Chapters 2.4 and 2.5. 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 2.1.8.

#### 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.

#### 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  $\mathcal{G}$  with respect to its translation subgroup. 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  $\mathcal{H} < \mathcal{G}$  in these tables are characterized by the elements of their general position. These elements are

# p2mg

Generators selected	(1); i	t(1,0);	t(0,1);	(2); (3)	)
---------------------	--------	---------	---------	----------	---

# General position

Multiplicity, Wyckoff letter, Site symmetry

# 4 *d* 1

Coordinates

(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	1,0
[2] p211 (2, p2)	1; 2		

# II Maximal klassengleiche subgroups

<ul> <li>Enlarged unit cell</li> </ul>			
[2] $b' = 2b$			
p2gg (8)	(2; 3+(0,1))	<b>a</b> ,2 <b>b</b>	
p2gg (8)	$\langle (2; 3) + (0, 1) \rangle$	<b>a</b> ,2 <b>b</b>	0, 1/2
p2mg (7)	$\langle 2; 3 \rangle$	<b>a</b> ,2 <b>b</b>	
p2mg (7)	$\langle 3; 2 + (0,1) \rangle$	<b>a</b> ,2 <b>b</b>	0, 1/2
[3] $a' = 3a$			
(p2mg (7))	(2; 3+(1,0))	3 <b>a</b> , <b>b</b>	
$\begin{cases} p2mg(7) \end{cases}$	(2+(2,0); 3+(3,0))	3 <b>a</b> , <b>b</b>	1,0
$p_{2mg}(7)$	(2+(4,0); 3+(5,0))	3 <b>a</b> , <b>b</b>	2,0
[3] $b' = 3b$			
(p2mg (7))	$\langle 2; 3 \rangle$	<b>a</b> ,3 <b>b</b>	
$\begin{cases} p2mg(7) \end{cases}$	$\langle 3; 2+(0,2) \rangle$	<b>a</b> ,3 <b>b</b>	0, 1
p2mg (7)	$\langle 3; 2+(0,4) \rangle$	<b>a</b> ,3 <b>b</b>	0,2
• Series of maximal	isomorphic subgroups		
$[p] \mathbf{a}' = p\mathbf{a}$			
p2mg (7)	$\langle 2 + (2u, 0); 3 + (\frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$	pa, b	<i>u</i> .0
rov	prime $p > 2$ : $0 < u < p$	<b>F</b> (1) (1)	
	<i>p</i> conjugate subgroups		
$[p] \mathbf{b}' = p\mathbf{b}$			
p2mg (7)	$\langle 3; 2+(0,2u) \rangle$	<b>a</b> , <i>p</i> <b>b</b>	0, <i>u</i>
	prime $p > 2$ ; $0 \le u < p$	<ul> <li>✓ ▲</li> </ul>	,

# I Minimal translationengleiche supergroups

none

# II Minimal non-isomorphic klassengleiche supergroups

*p* conjugate subgroups

# Additional centring translations

[2] *c*2*mm* (9)

# • Decreased unit cell

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

Cm	No. 8		A 1 1 m	
UNIQUE AXIS $c$ , CELL C	CHOICE 1			
<b>Generators selected</b> (1); <i>t</i>	t(1,0,0); t(0,1,0); t(0,0,1); t(0,	$(0, \frac{1}{2}, \frac{1}{2}); (2)$		
General position				
Multiplicity,		Coordin	ates	
Wyckoff letter, Site symmetry		(0,0,0)+ (0	$(0, \frac{1}{2}, \frac{1}{2}) +$	
4 <i>b</i> 1		(1) $x, y, z$ (	2) $x, y, \bar{z}$	
I Maximal translationenglei	che subgroups			
[2] A1 (1, P1)	1+		a, 1/2(b-c), 1/2(b+c))	<b>c</b> )
II Maximal klassengleiche s	ubgroups			
• Loss of centring translat	tions			
[2] P11b (7, P11a) [2] P11m (6)	1; 2+(0, $\frac{1}{2},\frac{1}{2}$ ) 1; 2		$\mathbf{b}, -\mathbf{a} - \mathbf{b}, \mathbf{c}$	0, 0, 1/4
• Enlarged unit cell				
$[2] \mathbf{a}' = 2\mathbf{a}$				
A11a (9) I11a (9, A11a) A11m (8) I11m (8 A11m)	$\begin{array}{c} \langle 2+(1,0,0) \rangle \\ \langle 2+(1,0,0) \rangle \\ \langle 2 \rangle \\ \langle 2 \rangle \end{array}$		2a, b, c 2a, $-2a + b$ , c 2a, b, c 2a $-2a + b$ c	
$[3] \mathbf{c}' = 3\mathbf{c}$	(-/		,, .	
$\begin{cases} A11m & (8) \\ A11m & (8) \\ A11m & (8) \end{cases}$ [3] $a' = 3a$	$egin{aligned} &\langle 2  angle \ &\langle 2+(0,0,2)  angle \ &\langle 2+(0,0,4)  angle \end{aligned}$		a,b,3c a,b,3c a,b,3c	$0, 0, 1 \\ 0, 0, 2$
$\begin{array}{c} A11m & (8) \\ \hline 3 & \mathbf{a}' = 3\mathbf{a}, \ \mathbf{b}' = -2\mathbf{a} + \mathbf{b} \end{array}$	$\langle 2 \rangle$		3 <b>a</b> , <b>b</b> , <b>c</b>	
A11m (8) [3] $\mathbf{a}' = 3\mathbf{a}, \ \mathbf{b}' = -4\mathbf{a} + \mathbf{b}$	$\langle 2 \rangle$		$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$	
A11 <i>m</i> (8) [3] $\mathbf{b}' = 3\mathbf{b}$	$\langle 2 \rangle$		$3\mathbf{a}, -4\mathbf{a} + \mathbf{b}, \mathbf{c}$	
A11m (8)	$\langle 2 \rangle$		<b>a</b> ,3 <b>b</b> , <b>c</b>	
• Series of maximal isomo	orphic subgroups			
$[p] \mathbf{c}' = p\mathbf{c}$ $A11m (8)$	$\langle 2 + (0, 0, 2u) \rangle$ prime $p > 2; \ 0 \le u < p$		<b>a</b> , <b>b</b> , <i>p</i> <b>c</b>	0,0, <i>u</i>
[n] a' = na b' = 2aa + b	p conjugate subgroups			
$[p] \mathbf{a} - p\mathbf{a}, \mathbf{b} = -2q\mathbf{a} + \mathbf{b}$ A11m (8)	$\langle 2 \rangle$ p prime; $0 \le q < p$ no conjugate subgroups		$p\mathbf{a}, -2q\mathbf{a}+\mathbf{b}, \mathbf{c}$	
$[p] \mathbf{b}' = p\mathbf{b}$				
A11m (8)	$\langle 2 \rangle$ prime $p > 2$ no conjugate subgroups		<b>a</b> , p <b>b</b> , <b>c</b>	

# I Minimal translationengleiche supergroups

II Minimal non-isomorphic klassengleiche supergroups

# • Additional centring translations

• Decreased unit cell

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

none

~5

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)

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

# I Maximal translationengleiche subgroups

[2] <i>Ib</i> 2 <i>m</i> (46, <i>Ima</i> 2) [2] <i>I</i> 2 <i>am</i> (46, <i>Ima</i> 2) [2] <i>Iba</i> 2 (45)	(1; 3; 6; 8) + (1; 4; 6; 7) + (1; 2; 7; 8) +	c,a,b c,b,-a	$0, 0, 1/4 \\ 0, 0, 1/4$
$ \begin{array}{l} [2] \ Iba2 \ (43) \\ [2] \ I222 \ (23) \\ [2] \ I12/a1 \ (15, C12/c1) \\ [2] \ I2/b11 \ (15, C12/c1) \\ [2] \ I112/m \ (12, A112/m) \end{array} $	(1, 2, 7, 8) + (1; 2; 3; 4) + (1; 3; 5; 7) + (1; 4; 5; 8) + (1; 2; 5; 6) +	$\mathbf{a} - \mathbf{c}, \mathbf{b}, \mathbf{c}$ $-\mathbf{b} - \mathbf{c}, \mathbf{a}, \mathbf{c}$ $\mathbf{b}, -\mathbf{a} - \mathbf{b}, \mathbf{c}$	0,0,1/4
II Maximal klassengleiche s	ubgroups		
• Loss of centring translat	tions		
[2] Pcan (60, Pbcn)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	- <b>b</b> , <b>a</b> , <b>c</b>	
[2] <i>Pbcn</i> (60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		
[2] <i>Pbcm</i> (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] <i>Pcam</i> (57, <i>Pbcm</i> )	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	- <b>b</b> , <b>a</b> , <b>c</b>	1/4, 1/4, 1/4
[2] <i>Pccn</i> (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] <i>Pbam</i> (55)	1; 2; 3; 4; 5; 6; 7; 8		
[2] <i>Pban</i> (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] <i>Pccm</i> (49)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		
• Enlarged unit cell			
[3] $a' = 3a$			
( <i>Ibam</i> (72)	$\langle 2; 5; 3+(1,0,0) \rangle$	3 <b>a</b> , <b>b</b> , <b>c</b>	
$\begin{cases} Ibam (72) \\ H (72) \end{cases}$	$\langle (2; 5) + (2,0,0); 3 + (3,0,0) \rangle$	3 <b>a</b> , <b>b</b> , <b>c</b>	1, 0, 0
(1bam (72))	$\langle (2; 5) + (4, 0, 0); 3 + (5, 0, 0) \rangle$	3 <b>a</b> , <b>b</b> , <b>c</b>	2,0,0
[5] <b>0</b> = 5 <b>0</b> ( <i>Ibam</i> (72)	(2: 5: 3 + (0 1 0))	a 3h c	
$\begin{cases} 1bam (72) \\ Ibam (72) \end{cases}$	$\langle (2; 5) + (0, 2, 0); 3 + (0, 1, 0) \rangle$	a, 3b, c	0.1.0
<i>Ibam</i> (72)	$\langle (2; 5) + (0, 4, 0); 3 + (0, 1, 0) \rangle$	<b>a</b> ,3 <b>b</b> , <b>c</b>	0, 2, 0
[3] $c' = 3c$			
$\int Ibam (72)$	$\langle 2; 3; 5 \rangle$	a, b, 3c	0.0.1
$\begin{cases} Ibam (72) \\ Ibam (72) \end{cases}$	$\langle 2; (3; 5) + (0, 0, 2) \rangle$	a, b, 3c	0, 0, 1
( <i>Ibam</i> ( <i>12</i> )	$\langle 2; (3; 5) + (0, 0, 4) \rangle$	a, d, 3c	0,0,2
• Series of maximal isomo	orphic subgroups		
$[p] \mathbf{a}' = p\mathbf{a}$	((2, 5) + (2, 0, 0), 2 + (p - 1 + 2, 0, 0))	and have	
10am (12)	$((2; 5) + (2u, 0, 0); 5 + (\frac{1}{2} - \frac{1}{2} + 2u, 0, 0))$ prime $p > 2; 0 \le u < p$ p conjugate subgroups	<i>р</i> а, <b>b</b> , <b>c</b>	<i>u</i> ,0,0
$[p] \mathbf{b}' = p\mathbf{b}$	/(2, 5) + (0, 2, 0), 2 + (0, p - 1, 0))	a mh a	0 0
10am (72)	$((2, 5) + (0, 2u, 0); 5 + (0, \frac{1}{2} - \frac{1}{2}, 0))$ prime $p > 2; 0 \le u < p$ p conjugate subgroups	a, <i>p</i> b,c	0, <i>u</i> , 0
$[p] \mathbf{c}' = p\mathbf{c}$			
Ibam (72)	$\langle 2; (3; 5) + (0, 0, 2u) \rangle$ prime $p > 2; 0 \le u < p$ p conjugate subgroups	<b>a</b> , <b>b</b> , <i>p</i> <b>c</b>	0,0, <i>u</i>

# I Minimal *translationengleiche* supergroups

[2] *I*4/*mcm* (140)

# II Minimal non-isomorphic klassengleiche supergroups

# • Additional centring translations

• 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*)

# *P*3*m*1

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

Gene	ral po	sition			
Multij Wyck Site sy	plicity, off lette ymmetr	r, y		Coordinates	3
6	е	1	(1) $x, y, z$ (4) $\bar{y}, \bar{x}, z$	(2) $\bar{y}, x - y, z$ (5) $\bar{x} + y, y, z$	(3) $\bar{x} + y, \bar{x}, z$ (6) $x, x - y, z$

### I Maximal translationengleiche subgroups

[2] P311 (143, P3)	1; 2; 3	
$\begin{bmatrix} 3 \end{bmatrix} P1m1 \ (8, C1m1)$	1; 4	-a+b, -a-b, 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

<ul> <li>Enlarged unit cell</li> </ul>			
[2] $c' = 2c$			
P3c1 (158)	$\langle 2; 4 + (0,0,1) \rangle$	<b>a</b> , <b>b</b> ,2 <b>c</b>	
P3m1 (156)	$\langle 2; 4 \rangle$	<b>a</b> , <b>b</b> , 2 <b>c</b>	
[3] $c' = 3c$			
P3m1 (156)	$\langle 2; 4 \rangle$	<b>a</b> , <b>b</b> ,3 <b>c</b>	
[3] $a' = 3a, b' = 3b$			
(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
$(H3m1 \ (157, P31m))$	$\langle 2+(2,1,0); 4+(2,2,0) angle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	1, 1, 0
(H3m1 (157, P31m)	$\langle 4; 2+(1,0,0)  angle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	2/3, -2/3, 0
$\begin{cases} H3m1 \ (157, P31m) \end{cases}$	$\langle 2\!+\!(2,2,0);4\!+\!(1,1,0) angle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	2/3, 1/3, 0
$(H3m1 \ (157, P31m))$	$\langle 2\!+\!(3,4,0);4\!+\!(2,2,0) angle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	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
$\begin{cases} H3m1 \ (157, P31m) \end{cases}$	$\langle 2+(2,3,0); 4+(1,1,0)  angle$	$\mathbf{a} - \mathbf{b}, \mathbf{a} + 2\mathbf{b}, \mathbf{c}$	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 <b>a</b> ,2 <b>b</b> , <b>c</b>	
P3m1 (156)	$\langle 2+(1,-1,0); 4+(1,1,0) \rangle$	2 <b>a</b> ,2 <b>b</b> , <b>c</b>	1, 0, 0
P3m1 (156)	(2+(1,2,0); 4+(1,1,0))	2 <b>a</b> ,2 <b>b</b> , <b>c</b>	0,1,0
(P3m1 (156))	$\langle 2+(2,1,0); 4+(2,2,0) \rangle$	2 <b>a</b> ,2 <b>b</b> , <b>c</b>	1,1,0
• Series of maximal isom	orphic subgroups		
$[p] \mathbf{c}' = p\mathbf{c}$			
P3m1 (156)	$\langle 2; 4 \rangle$	<b>a</b> , <b>b</b> , <i>p</i> <b>c</b>	
	<i>p</i> prime	· · · •	
	no conjugate subgroups		
$[p^2] \mathbf{a}' = p\mathbf{a}, \ \mathbf{b}' = p\mathbf{b}$			
<i>P</i> 3 <i>m</i> 1 (156)	$\langle 2 + (u + v, -u + 2v, 0); 4 + (u + v, u + v, 0) \rangle$ prime $p \neq 3; 0 \le u < p; 0 \le v < p$ $p^2$ conjugate subgroups	p <b>a</b> , p <b>b</b> , <b>c</b>	<i>u</i> , <i>v</i> ,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]  $R_{obv}3m$  (160, R3m); [3]  $R_{rev}3m$  (160, R3m)

• Decreased unit cell

No. 222

# 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

Mult Wycl Site s	iplicity koff let symme	y, tter, etry		Coord	linates	
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) $y, \overline{z}, \overline{x}$	(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) $x, z, \overline{y}$	(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) $x + \frac{1}{2}, y + \frac{1}{2}, \overline{z} + \frac{1}{2}$	(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) $y + \frac{1}{2}, \overline{z} + \frac{1}{2}, x + \frac{1}{2}$	(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) $\bar{y} + \frac{\bar{1}}{2}, \bar{x} + \frac{\bar{1}}{2}, z + \frac{\bar{1}}{2}$	(38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	(39) $\bar{y} + \frac{\bar{1}}{2}, x + \frac{\bar{1}}{2}, \bar{z} + \frac{\bar{1}}{2}$	(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) $x + \frac{\bar{1}}{2}, \bar{z} + \frac{\bar{1}}{2}, \bar{y} + \frac{\bar{1}}{2}$	(43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(44) $\bar{x} + \frac{\bar{1}}{2}, z + \frac{\bar{1}}{2}, \bar{y} + \frac{\bar{1}}{2}$
			(45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(46) $\bar{z} + \frac{\bar{1}}{2}, y + \frac{\bar{1}}{2}, \bar{x} + \frac{\bar{1}}{2}$	(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		
$\int [3] P4/n12/n (126, P4/nnc)$	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42;	b,c,a	
	43; 41; 44		
[3] P4/n12/n (126, P4/nnc)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46;	<b>c</b> , <b>a</b> , <b>b</b>	
	48; 47; 45		
$\left( \begin{bmatrix} 4 \end{bmatrix} P \hat{132} / n \ (167, R \hat{3}c) \right)$	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
$1$ [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

# • Series of maximal isomorphic subgroups

 $\begin{array}{ll} [p^3] \ \mathbf{a}' = p \mathbf{a}, \ \mathbf{b}' = p \mathbf{b}, \ \mathbf{c}' = p \mathbf{c} \\ Pn \overline{3}n \ (222) & \langle 2 + (2u, 2v, 0); \ 3 + (2u, 0, 2w); & p \mathbf{a}, p \mathbf{b}, p \mathbf{c} \\ 5 + (u - w, -u + v, -v + w); \\ 13 + (u - v, -u + v, 2w); \\ 25 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, \frac{p}{2} - \frac{1}{2} + 2w) \rangle \\ prime \ p > 2; \ 0 \le u < p; \ 0 \le v < p; \ 0 \le w < p \\ p^3 \ \text{conjugate subgroups} \end{array}$ 

# I Minimal translationengleiche supergroups

none

none

# II Minimal non-isomorphic klassengleiche supergroups

# • Additional centring translations

[2] *Im*3*m* (229); [4] *Fm*3*c* (226)

• Decreased unit cell

# Pn3n

 $P4/n\bar{3}2/n$ 

# 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

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

Coordinates

# 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;		1/4,1/4,1/4
	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;		1/4,1/4,1/4
[0] p 31 (001 p 3)	16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] Pn31 (201, Pn3)	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;	b,c,a	
	43; 41; 44		
[3] P4/n12/n (126, P4/nnc)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46;	<b>c</b> , <b>a</b> , <b>b</b>	
<u> </u>	48; 47; 45		
$([4] P1\bar{3}2/n (167, R\bar{3}c))$	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	-a + b, -b - c, -a - b + c	1/2, 1/2, 0
•			

 $\begin{array}{l} \langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);\\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0,\frac{p}{2}-\frac{1}{2}+2w);\\ 5+(u-w,-u+v,-v+w); \end{array}$ 

 $13 + (u - v, -u + v, \frac{p}{2} - \frac{1}{2} + 2w);$ 

prime p > 2;  $0 \le u < p$ ;  $0 \le v < p$ ;  $0 \le w < p$ 

 $25 + (2u, 2v, 2w)\rangle$ 

 $p^3$  conjugate subgroups

# II Maximal klassengleiche subgroups

• Enlarged unit cell

 $Pn\bar{3}n$  (222)

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

none

p**a**, p**b**, p**c** 

u, v, w

# I Minimal translationengleiche supergroups

• Series of maximal isomorphic subgroups

# II Minimal non-isomorphic klassengleiche supergroups

# • Additional centring translations

[2] *Im*3*m* (229); [4] *Fm*3*c* (226)

• Decreased unit cell

none

# 2. MAXIMAL SUBGROUPS OF THE PLANE GROUPS AND SPACE GROUPS



Fig. 2.4.1.5. Graph of the *translationengleiche* subgroups of the summit space group  $Fm\overline{3}m$  and of the included graphs with summits  $\mathcal{H} < Fm\overline{3}m$ , see Example 2.1.8.2.3.



Fig. 2.4.1.6. Graph of the *translationengleiche* subgroups of the summit space group  $Fm\overline{3}c$  and of the included graphs with summits  $\mathcal{H} < Fm\overline{3}c$ , see Example 2.1.8.2.3.

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

For an explanation of these graphs, see Section 2.1.8.3.







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 3*m*.

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

symbol change as given by the arrows, and simultaneously the labels change:

**abc**: 
$$P2/b2_1/c2_1/m$$
  $x, \frac{1}{4}, 0$   
**bca**:  $P2_1/b2_1/m2/a$   $\frac{1}{4}, 0, z$   
**bca**:  $P2_1/b2_1/m2/a$   $\frac{1}{4}, 0, z$   
**bac**:  $P2_1/c2_1/m$   $x, \frac{1}{4}, 0$   
**bac**:  $P2_1/c2_1/m$   $\frac{1}{4}, -y, 0$ 

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*.

The corresponding interchanges of positions and labels for all possible nonconventional settings are listed at the end of the table of each orthorhombic space group. They have to be applied to all subgroups.

#### Example 3.1.4.2

Consider the nonconventional setting *Pcam* of *Pbcm*. The entry at the bottom of the page for space group *Pbcm*, No. 57, shows the necessary interchanges for the setting *Pcam*:  $a \rightleftharpoons b$ ,  $\mathbf{a} \rightleftharpoons -\mathbf{b}$ , and  $x \rightleftharpoons -y$ .

For the subgroup *Pbna* (last entry in the block of *klassen-gleiche* non-isomorphic subgroups) this means: *Pbna* has to be replaced by *Pnab*, the axes conversion 2**a**, **b**, **c** has to be replaced by **a**,  $-2\mathbf{b}$ , **c** and the coordinate transformation  $\frac{1}{2}x + \frac{1}{4}$ , *y*, *z*;  $+(\frac{1}{2}, 0, 0)$  has to be replaced by *x*,  $-\frac{1}{2}y - \frac{1}{4}$ , *z*;  $+(0, -\frac{1}{2}, 0)$ .

Pbna and Pnab are nonconventional settings of Pbcn, No. 60.

The interchange of the axes does not affect the Wyckoff labels, just the corresponding coordinates.

#### Example 3.1.4.3

The Wyckoff position  $4c (x, \frac{1}{4}, 0)$  of *Pbcm*, No. 57, retains its label for any of the other settings of this space group. In the setting *Pbma*, this Wyckoff position is still 4c and has the coordinates  $\frac{1}{4}$ , 0, *z*. In this case, no ambiguity arises because the different settings of space group *Pbcm* all have different Hermann–Mauguin symbols that uniquely show how the axes have to be interchanged (*Pmca*, *Pbma*, *Pcam*, *Pmab* and *Pcmb*).

The interchange of the axes must also be performed for those subgroups that have equivalent directions and where the Hermann–Mauguin symbol does not uniquely show the kind of setting. Otherwise, the wrong Wyckoff positions can result.

#### Example 3.1.4.4

Space group *Cmmm*, No. 65, has two *klassengleiche* subgroups of type *Immm*, No. 71, with doubled *c* axis. In the nonconventional setting *Bmmm* of *Cmmm*, the same subgroups *Immm* result from a doubling of the *b* axis. In the conventional setting of *Immm*, the Wyckoff positions 4*e*, 4*g* and 4*i* represent orbits with the coordinates (x, 0, 0), (0, y, 0) and (0, 0, z), respectively. In the space group *Cmmm*, the position 4*k* corresponds to (0, 0, z) and upon transition to either of the subgroups *Immm* it splits to  $2 \times 4i$ .

If *Bmmm* is obtained from *Cmmm* by cyclic exchange of the axes ( $\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$ ), its Wyckoff position 4k obtains the coordinates (0, y, 0). Upon doubling of b and transition to *Immm*, 4k will split to two orbits with the coordinates (0,  $\frac{1}{2}y$ , 0) and (0,  $\frac{1}{2}y + \frac{1}{2}$ , 0). These are two orbits 4i of *Immm*, but this is only correct if the axes of *Immm* have also been interchanged in the same way. If the interchange of axes has not been performed in the subgroup Immm in the assumption that

in Immm all axes are equivalent anyway, wrong results will be obtained. That is, Immm also has to be used in a nonconventional setting, although this is not apparent from the Hermann-Mauguin symbol. Of course, the Wyckoff symbols can then be relabelled so that they correspond to the conventional listings of Volume A  $(4i \rightarrow 4g \ etc.)$ . It is recommended that this return to the conventional setting of Immm is performed, because using the label 4*i* for (0, y, 0) in Immm is likely to cause confusion if the nonconventional setting is not explicitly stressed.

#### 3.1.5. Conjugate subgroups

Conjugate subgroups are different subgroups belonging to the same space-group type (they have the same Hermann–Mauguin symbol) and they have the same unit-cell size and the same shape for the conventional cell. They can be mapped onto one another by a symmetry operation of the starting group, *i.e.* they are symmetry-equivalent in this space group. They can occur only if the index of symmetry reduction is  $\geq 3$ . The relations of the Wyckoff positions of a space group with the Wyckoff positions of any representative of a set of conjugate subgroups are always the same. Therefore, in principle it is sufficient to list the relations for only one representative.

Two kinds of conjugation of maximal subgroups can be distinguished, translational conjugation and orientational conjugation. Non-maximal subgroups can involve both kinds of conjugation, so the situation is more complicated in chains of group–subgroup relations, *cf.* Koch (1984) and Müller (1992). Since the present tables only list maximal subgroups, we will not discuss this here.

#### 3.1.5.1. Translational conjugation

Translational conjugation occurs when the group-subgroup relation involves a loss of translational symmetry. This happens when the conventional cell has been enlarged or when centring translations have been lost; this means that the primitive unit cell of the subgroup is larger (by a factor  $\geq 3$ ). Translationally conjugate subgroups of a space group are symmetry-equivalent by a translation of the lattice of this space group. This way, isomorphic subgroups of index  $p \ge 3$  have p conjugate subgroups (unless the cell enlargement occurs in a direction in which the origin may float). The existence of conjugate subgroups of this kind is not specifically mentioned in the tables. However, they can be recognized by looking in the column 'Coordinates'. If a semicolon appears after the coordinate triplet, followed by values in parentheses to be added, and if, in addition, the index of symmetry reduction is > 3, then conjugate subgroups usually exist. They differ in the locations of their origins by values corresponding to the values given in the parentheses.

#### Example 3.1.5.1.1

$$x, y, \frac{1}{3}z; \pm (0, 0, \frac{1}{3})$$

gives the positional coordinates in the subgroup originating from the coordinates of one unit cell of the starting group, namely

 $x, y, \frac{1}{3}z; \quad x, y, \frac{1}{3}z + \frac{1}{3}; \quad x, y, \frac{1}{3}z - \frac{1}{3}.$ 

In addition, this also means that there are three conjugate subgroups. They differ in the locations of their origins referred to the origin of the starting space group by  $0, 0, 0, 0, 0, \frac{1}{3}$  and

# *Cm C*1*m*1 No. 8

A1m1

**CELL CHOICE 2** 



CELL CHOICE 3

UNIQUE AXIS *b* CELL CHOICE 1

#### Coordi-Wyckoff positions Coordi-Coordi-Axes Axes Axes nates 2a4bnates nates I Maximal translation engleiche subgroups [2] P1 (1) $\frac{1}{2}(\mathbf{a}-\mathbf{b}),$ 1a $2 \times 1a$ P1 a.b. *P*1 2x, x+y, z;x, x+y, 2za. x+y, 2y, y+zb. c $\frac{1}{2}(-b+c)$ $\frac{1}{2}(-a+b-c), c$ II Maximal klassengleiche subgroups Loss of centring translations [2] P1a1 (7) $x, y + \frac{1}{4}, z$ 2a $2 \times 2a$ P1c1 $x, y + \frac{1}{4}, z$ P1n1 $x, y + \frac{1}{4}, z$ [2] *P*1*m*1 (6) 1a; 1b $2 \times 2c$ P1m1P1m1Enlarged unit cell, non-isomorphic [2] *C*1*c*1 (9) **a**, **b**, 2**c** $2 \times 4a$ A1n1 $2\mathbf{a}+\mathbf{c}$ , $\frac{1}{2}x, y, -\frac{1}{2}x+z;$ I1a12**a**, **b**, $\frac{1}{2}(x+z), y, z;$ $x, y, \frac{1}{2}z;$ 4ab, c $+(\frac{1}{2},0,0)$ $+(0,0,\frac{1}{2})$ $+(\frac{1}{2},0,0)$ -a+c [2] C1c1 (9) **a**-2**c**, **b**, 2**c** $x, y, x+\frac{1}{2}z;$ 4a $2 \times 4a$ I1a12a, b, c $\frac{1}{2}x, y, z;$ I1a12**a**, **b**, $\frac{1}{2}(x-z), y, z;$ $+(0,0,\frac{1}{2})$ $+(\frac{1}{2},0,0)$ $+(\frac{1}{2},0,0)$ a+c $x, y + \frac{1}{4}, \frac{1}{2}z;$ $\hat{=} I1a1$ **a**, **b**, 2**c** $+(0,0,\frac{1}{2})$ Enlarged unit cell, isomorphic [3] C1m1 a, 3b, c $x, \frac{1}{3}y, z;$ 2a; 4b $3 \times 4b$ A1m1 a, 3b, c $x, \frac{1}{3}y, z;$ *I*1*m*1 **a**, 3**b**, **c** $x, \frac{1}{3}y, z;$ $\pm (0, \frac{1}{3}, 0)$ $\pm (0, \frac{1}{3}, 0)$ $\pm (0, \frac{1}{3}, 0)$ $2a; \frac{p-1}{2} \times 4b p \times 4b$ A1m1 **a**, p**b**, **c** $x, \frac{1}{n}y, z;$ [p] C1m1 $x, \frac{1}{n}y, z;$ $x, \frac{1}{n}y, z;$ **a**, *p***b**, **c** *I*1*m*1 **a**, *p***b**, **c** $+(0,\frac{u}{n},0)$ $+(0,\frac{u}{n},0)$ $+(0,\frac{u}{n},0)$ $p = \text{prime} > 2; u = 1, \dots, p-1$ $p = \text{prime} > 2; u = 1, \dots, p-1$ $p = \text{prime} > 2; u = 1, \dots, p-1$ $\frac{1}{2}x, y, z;$ [2] C1m1 **a**, **b**, 2**c** $x, y, \frac{1}{2}z;$ $2 \times 2a$ $2 \times 4b$ A1m1 2a, b, c I1m1 2a, b, -a+c $\frac{1}{2}(x+z), y, z;$ $+(0,0,\frac{1}{2})$ $+(\frac{1}{2},0,0)$ $+(\frac{1}{2},0,0)$ [2] *I*1*m*1 a, b, 2c $x, y, \frac{1}{2}z;$ $2 \times 2a$ $2 \times 4b$ *I*1*m*1 2**a**, **b**, **c** $\frac{1}{2}x, y, z;$ *I*1*m*1 2**a**, **b**, **a**+**c** $\frac{1}{2}(x-z), y, z;$ $+(0,0,\frac{1}{2})$ $+(\frac{1}{2},0,0)$ $+(\frac{1}{2},0,0)$ 3a, b, c $\frac{1}{2}x, y, z;$ $3 \times 2a$ $3 \times 4b$ A1m1 $\mathbf{a}+\mathbf{c}$ , $x, y, \frac{1}{3}(-x+z);$ $x, y, \frac{1}{3}z;$ [3] C1m1 *I*1*m*1 **a**, **b**, 3**c** $\pm(\frac{1}{3},0,0)$ $\pm (0,0,\frac{1}{3})$ $\pm (0,0,\frac{1}{3})$ **b**, 3**c** [3] C1m1 $\frac{1}{3}(x+z), y, z; |3 \times 2a|$ $3 \times 4b$ A1m1 $\mathbf{a}-\mathbf{c}$ , $x, y, \frac{1}{3}(x+z);$ *I*1*m*1 3**a**, **b**, $\frac{1}{3}(x-2z), y, z;$ 3**a**, **b**, $\pm(\frac{1}{3},0,0)$ **b**, 3**c** $\pm (0,0,\frac{1}{3})$ 2**a+c** $\pm(\frac{1}{3},0,0)$ -a+c [3] C1m1 3**a**, **b**, $\frac{1}{3}(x-z), y, z;$ $3 \times 2a$ $3 \times 4b$ A1m1 **a**, **b**, 3**c** $x, y, \frac{1}{3}z;$ *I*1*m*1 3**a**, **b**, **c** $\frac{1}{3}x, y, z;$ $\pm(\frac{1}{3},0,0)$ $\pm (0,0,\frac{1}{3})$ $\pm(\frac{1}{3},0,0)$ a+c [3] C1m1 a, b, 3c $x, y, \frac{1}{3}z;$ $3 \times 2a$ $3 \times 4b$ A1m1 3a, b, c $\frac{1}{2}x, y, z;$ *I*1*m*1 3**a**, **b**, $\frac{1}{2}(x+2z), y, z;$ $\pm (0,0,\frac{1}{3})$ $+(\frac{1}{3},0,0)$ $-2\mathbf{a}+\mathbf{c}$ $\pm(\frac{1}{3},0,0)$ **a**, **b**, *p***c** $x, y, \frac{1}{p}z;$ [*p*] *C*1*m*1 $p \times 2a$ $p \times 4b$ A1m1 pa, b, c $\frac{1}{n}x, y, z;$ *I*1*m*1 *p***a**, **b**, **c** $\frac{1}{n}x, y, z;$ $+(0,0,\frac{u}{p})$ $+(\frac{u}{n},0,0)$ $\pm(\frac{u}{n}, 0, 0)$ p = prime; u = 1, ..., p - 1p = prime; u = 1, ..., p-1 $p = \text{prime}; > 2; u = 1, \dots, p-1$ [p] C1m1 $\frac{1}{p}(x-qz), y, z; p \times 2a$ $p \times 4b$ $x, y, \frac{1}{p}(-qx+z);$ I1m1 $\mathbf{a}+2q\mathbf{c}$ , $x, y, \frac{1}{p}(-2qx+z);$ *p***a**. **b**. A1m1 $\mathbf{a}+q\mathbf{c}$ , $+(\frac{u}{p},0,0)$ $+(0,0,\frac{u}{p})$ $+(0,0,\frac{u}{p})$ $q\mathbf{a} + \mathbf{c}$ **b**, *p***c** b, pc $p = \text{prime} > 2; u = 1, \dots, p-1;$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $p = \text{prime} > 2; u = 1, \dots, p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$

 $26 \\ 2h$ 

I2/b2/a2/m

No. 72

Ibam

	Axes	Coordinates					Wy	ckoff po	sitions				
			4a	4b	4c	4d	8 <i>e</i>	8 <i>f</i>	8 <i>g</i>	8h	8 <i>i</i>	8 <i>j</i>	16k
I Maximal tr	anslationen	<i>gleiche</i> subgroups					_						
$\begin{array}{c} [2] I2cm (46) \\ \widehat{=} Ima2 \end{array}$	c, -b, a	$x, y, z + \frac{1}{4}$ $z + \frac{1}{4}, -y, x$	4 <i>a</i>	4 <i>a</i>	4 <i>b</i>	4 <i>b</i>	8 <i>c</i>	$2 \times 4a$	8 <i>c</i>	8 <i>c</i>	8 <i>c</i>	$2 \times 4b$	$2 \times 8c$
$[2] Ic2m (46)$ $\widehat{=} Ima2$	c, a, b	$x, y, z + \frac{1}{4}$ $z + \frac{1}{4}, x, y$	4 <i>a</i>	4 <i>a</i>	4 <i>b</i>	4 <i>b</i>	8 <i>c</i>	8 <i>c</i>	$2 \times 4a$	8 <i>c</i>	8 <i>c</i>	$2 \times 4b$	$2 \times 8c$
[2] <i>Iba</i> 2 (45)			4 <i>a</i>	4b	4 <i>a</i>	4 <i>b</i>	8 <i>c</i>	8 <i>c</i>	8 <i>c</i>	$2 \times 4a$	$2 \times 4b$	8 <i>c</i>	$2 \times 8c$
[2] 1222 (23)		$x, y, z + \frac{1}{4}$	2a;2c	2b;2d	4 <i>i</i>	4 <i>j</i>	8 <i>k</i>	4e;4f	4g; 4h	$2 \times 4i$	$2 \times 4j$	8 <i>k</i>	$2 \times 8k$
[2] I2/c11 (15)  = I12/a1  = C12/c1	c, a, b -b-c. a. c	z, x, y -y, x, -y+z	4 <i>e</i>	4 <i>e</i>	4 <i>a</i>	4 <i>b</i>	4c;4d	2×4 <i>e</i>	8 <i>f</i>	8 <i>f</i>	8 <i>f</i>	8 <i>f</i>	$2 \times 8f$
[2] I12/c1 (15)  = C12/c1	a–c, b, c	<i>x</i> , <i>y</i> , <i>x</i> + <i>z</i>	4 <i>e</i>	4 <i>e</i>	4 <i>a</i>	4 <i>b</i>	4 <i>c</i> ;4 <i>d</i>	8 <i>f</i>	2×4 <i>e</i>	8 <i>f</i>	8 <i>f</i>	8 <i>f</i>	$2 \times 8f$
$\begin{array}{c} [2] I112/m(12) \\ \widehat{=} A112/m \end{array}$	b, -a-b, c	-x+y,-y,z	4 <i>g</i>	4 <i>h</i>	2a;2b	2c;2d	4 <i>e</i> ;4 <i>f</i>	8 <i>j</i>	8 <i>j</i>	$2 \times 4g$	$2 \times 4h$	$2 \times 4i$	$2 \times 8j$
II Maximal k Loss of cer	<i>lassengleich</i> ntring transl	<i>e</i> subgroups lations											
[2] <i>Pbcn</i> (60)			4 <i>c</i>	4c	4a	4b	8 <i>d</i>	8 <i>d</i>	$2 \times 4c$	8 <i>d</i>	8 <i>d</i>	8 <i>d</i>	$2 \times 8d$
[2] <i>Pcan</i> (60)	b, -a, c	<i>y</i> , <i>-x</i> , <i>z</i>	4 <i>c</i>	4 <i>c</i>	4 <i>a</i>	4 <i>b</i>	8 <i>d</i>	$2 \times 4c$	8 <i>d</i>	8 <i>d</i>	8 <i>d</i>	8 <i>d</i>	$2 \times 8d$
[2] <i>Pbcm</i> (57)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	4 <i>c</i>	4 <i>c</i>	4d	4 <i>d</i>	4a;4b	$2 \times 4c$	8 <i>e</i>	8 <i>e</i>	8 <i>e</i>	$2 \times 4d$	$2 \times 8e$
[2] <i>Pcam</i> (57)	b, -a, c	$ \begin{array}{c} x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4} \\ y + \frac{1}{4}, -x - \frac{1}{4}, z + \frac{1}{4} \end{array} $	4 <i>c</i>	4 <i>c</i>	4 <i>d</i>	4 <i>d</i>	4 <i>a</i> ;4b	8 <i>e</i>	$2 \times 4c$	8 <i>e</i>	8 <i>e</i>	$2 \times 4d$	$2 \times 8e$
[2] <i>Pccn</i> (56)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	4 <i>c</i>	4d	4 <i>c</i>	4d	4a;4b	8 <i>e</i>	8 <i>e</i>	$2 \times 4c$	$2 \times 4d$	8 <i>e</i>	$2 \times 8e$
[2] <i>Pbam</i> (55)			4 <i>e</i>	4f	2a; 2b	2c;2d	8 <i>i</i>	8 <i>i</i>	8 <i>i</i>	$2 \times 4e$	$2 \times 4f$	4g;4h	$2 \times 8i$
[2] <i>Pban</i> (50)	origin 1: origin 2:	$x, y, z + \frac{1}{4} x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	2a;2d	2b;2c	4 <i>k</i>	41	4e;4f	4g; 4h	4 <i>i</i> ;4 <i>j</i>	$2 \times 4k$	$2 \times 4l$	8 <i>m</i>	2×8 <i>m</i>
[2] <i>Pccm</i> (49)			2e;2h	2f; 2g	2a; 2b	2c;2d	8 <i>r</i>	4 <i>i</i> ;4 <i>j</i>	4k;4l	4 <i>m</i> ;4 <i>n</i>	4 <i>o</i> ;4 <i>p</i>	$2 \times 4q$	$2 \times 8r$
Enlarged u	ınit cell, isoı	morphic											
[3] <i>Ibam</i>	3 <b>a</b> , <b>b</b> , <b>c</b>	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	4 <i>a</i> ;8 <i>f</i>	4 <i>b</i> ;8 <i>f</i>	4 <i>c</i> ;8 <i>j</i>	4 <i>d</i> ;8 <i>j</i>	8e;16k	$3 \times 8f$	8g;16k	8 <i>h</i> ;16 <i>k</i>	8 <i>i</i> ;16 <i>k</i>	$3 \times 8j$	$3 \times 16k$
[p] Ibam	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$ p = prime >	$\frac{\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)}{2; u = 1, \dots, p-1}$	$4a;$ $\frac{p-1}{2} \times 8f$	$\frac{4b}{\frac{p-1}{2}\times}$	$4c;$ $\frac{p-1}{2} \times 8i$	$\frac{4d}{\frac{p-1}{2}\times}$	$\frac{8e;}{\frac{p-1}{2}\times}$	p×8f	$8g;$ $\frac{p-1}{2} \times 16k$	$\frac{8h}{\frac{p-1}{2}\times}$	$8i;$ $\frac{p-1}{2} \times 16k$	p×8j	<i>p</i> ×16 <i>k</i>
[3] <i>Ibam</i>	<b>a</b> , 3 <b>b</b> , <b>c</b>	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	4 <i>a</i> ;8 <i>g</i>	4 <i>b</i> ;8 <i>g</i>	4 <i>c</i> ;8 <i>j</i>	4d;8j	8e;16k	8 <i>f</i> ;16k	$3 \times 8g$	8 <i>h</i> ;16 <i>k</i>	8 <i>i</i> ;16 <i>k</i>	3×8j	3×16 <i>k</i>
[p] Ibam	<b>a</b> , p <b>b</b> , <b>c</b>	$x, \frac{1}{n}y, z; +(0, \frac{u}{n}, 0)$	4 <i>a</i> ;	4 <i>b</i> ;	4 <i>c</i> ;	4 <i>d</i> ;	8e;	8 <i>f</i> ;	$p \times 8g$	8 <i>h</i> ;	8 <i>i</i> ;	$p \times 8j$	$p \times 16k$
	p = prime >	> 2; $u = 1, \dots, p-1$	$\frac{p-1}{2} \times 8g$	$\frac{p-1}{2} \times 8g$	$\frac{p-1}{2} \times 8j$	$\frac{p-1}{2} \times 8j$	$\frac{p-1}{2} \times 16k$	$\frac{p-1}{2} \times 16k$		$\frac{p-1}{2} \times 16k$	$\frac{p-1}{2} \times 16k$		
[3] <i>Ibam</i>	a, b, 3c	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	4 <i>a</i> ;8 <i>h</i>	4 <i>b</i> ;8 <i>i</i>	4 <i>c</i> ;8 <i>h</i>	4 <i>d</i> ;8 <i>i</i>	8e;16k	8 <i>f</i> ;16 <i>k</i>	8g;16k	$3 \times 8h$	$3 \times 8i$	8 <i>j</i> ;16k	$3 \times 16k$
[p] Ibam	<b>a</b> , <b>b</b> , <i>p</i> <b>c</b> <i>p</i> = prime >	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ > 2; $u = 1, \dots, p-1$	$\begin{array}{c}4a;\\\frac{p-1}{2}\times\\8h\end{array}$	$\begin{array}{c}4b;\\\frac{p-1}{2}\times\\8i\end{array}$	$\begin{array}{c} 4c; \\ \frac{p-1}{2} \times \\ 8h \end{array}$	$\begin{array}{c} 4d;\\ \frac{p-1}{2}\times\\ 8i \end{array}$	$\frac{8e;}{\frac{p-1}{2}\times}$	$\frac{8f;}{\frac{p-1}{2}\times}$	$\frac{p-1}{2} \times \frac{16k}{16k}$	$p \times 8h$	p×8i	$8j;$ $\frac{p-1}{2} \times 16k$	<i>p</i> ×16 <i>k</i>

# Nonconventional settings

Interchange letters and sequences in Hermann-Mauguin symbols, axes and coordinates:

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

# P3m1

		Axes	Coordinates		Wycko	ff positions		
				1 <i>a</i>	1 <i>b</i>	1 <i>c</i>	3 <i>d</i>	6e
Ι	Maximal	translationengl	eiche subgroups					
[2]	P3 (143)			1 <i>a</i>	1 <i>b</i>	1 <i>c</i>	3 <i>d</i>	$2 \times 3d$
[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	$3 \times 4b$
	conjugate:	a−b, a+b, c	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$		1	1		
	conjugate:	a+2b, −a, c	$\frac{1}{2}y, -x + \frac{1}{2}y, z$					
II	Maximal	klassengleiche	subgroups					
	Enlarged	unit cell, non-i	somorphic					
[2]	P3c1	<b>a</b> , <b>b</b> , 2 <b>c</b>	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	2a	2b	2c	6 <i>d</i>	$2 \times 6d$
	(158)							
[3]	P31m	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$	1 <i>a</i> ;2 <i>b</i>	3 <i>c</i>	3 <i>c</i>	3c;6d	$3 \times 6d$
	(157)		$\pm(\frac{2}{3},\frac{1}{3},0)$					
[3]	P31m	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3},\frac{1}{3}(-x+2y),z;$	3 <i>c</i>	1 <i>a</i> ;2 <i>b</i>	3 <i>c</i>	3c;6d	$3 \times 6d$
[0]	(157)		$\pm(\frac{2}{3},\frac{1}{3},0)$	2	2	1 01		
[3]	P31m (157)	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3},\frac{1}{3}(-x+2y),z;$ + $(\frac{2}{3},\frac{1}{3},0)$	3 <i>c</i>	3 <i>c</i>	1 <i>a</i> ;2 <i>b</i>	3c;6d	$3 \times 6d$
	(157)		$\perp(\frac{1}{3},\frac{1}{3},0)$					
	Enlarged	unit cell, isomo	orpnic					
[2]	<i>P</i> 3 <i>m</i> 1	<b>a</b> , <b>b</b> , 2 <b>c</b>	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2 \times 1a$	$2 \times 1b$	$2 \times 1c$	$2 \times 3d$	$2 \times 6e$
[3]	P3m1	a, b, 3c	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3 \times 1a$	$3 \times 1b$	$3 \times 1c$	$3 \times 3d$	3×6 <i>e</i>
[ <i>p</i> ]	P3m1	<b>a</b> , <b>b</b> , <i>p</i> <b>c</b>	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p \times 1a$	$p \times 1b$	$p \times 1c$	$p \times 3d$	$p \times 6e$
		p = prime; $u =$	1,, p-1					
[4]	P3m1	2 <b>a</b> , 2 <b>b</b> , <b>c</b>	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0);$	1 <i>a</i> ;3 <i>d</i>	1 <i>c</i> ;3 <i>d</i>	1 <i>b</i> ;3 <i>d</i>	$2 \times 3d$ ;6 $e$	$4 \times 6e$
			$+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$					
$[p^2]$	<i>P</i> 3 <i>m</i> 1	p <b>a</b> , p <b>b</b> , <b>c</b>	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$1a;(p-1)\times 3d;$	$1b(c^{*});$	$1c(b^{*});$	$p \times 3d;$	$p^2 \times 6e$
		$p = \text{prime} \neq 3$	; $u, v = 1, \dots, p-1$	$\frac{(p-1)(p-2)}{6} \times 6e$	$(p-1)\times 3d;$	$(p-1)\times 3d;$	$\frac{p(p-1)}{2} \times 6e$	
					$\frac{(p-1)(p-2)}{6} \times 6e$	$\frac{(p-1)(p-2)}{6} \times 6e$		

\* p = 3n - 1

# $Pn\bar{3}n$

 $P4/n\bar{3}2/n$ 

 $O_h^2$ 

Axes	Coordinates		Wyckoff positions					
	origin 1	origin 2	2 <i>a</i>	6 <i>b</i>	8 <i>c</i>	12 <i>d</i> 24 <i>g</i>	12e 24h	16 <i>f</i> 48 <i>i</i>
I Maximal translation	engleiche subg	roups	•	•	•	•	•	•
[2] <i>P</i> 43 <i>n</i> (218)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	2 <i>a</i>	6 <i>b</i>	8e	6c;6d 12g;12h	12 <i>f</i> 24 <i>i</i>	$2 \times 8e \\ 2 \times 24i$
[2] <i>P</i> 432 (207)		$x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	1 <i>a</i> ;1 <i>b</i>	3c;3d	8 <i>g</i>	$12h \\ 2 \times 12h$	6e;6f 12i;12j	$2 \times 8g$ $2 \times 24k$
[2] <i>Pn</i> 3 (201)			2a	6 <i>d</i>	4 <i>b</i> ;4 <i>c</i>	12g 2×12g	12 <i>f</i> 24 <i>h</i>	$2 \times 8e$ $2 \times 24h$
$[4] R\bar{3}c$ (167) ( rhombohed	$x - \frac{1}{4}, y - \frac{1}{4}, z - \frac{1}{4}$ ral axes)		2a	6 <i>e</i>	2b;6d	$\begin{array}{c} 12f\\ 2\times 12f \end{array}$	12 <i>f</i> 2×6 <i>e</i> ;12 <i>f</i>	4 <i>c</i> ;12 <i>f</i> 4×12 <i>f</i>
$\begin{array}{c} \mathbf{a-b, b-c,} \\ \mathbf{a+b+c} \\ (hex. axes) \\ \text{conjugate: } -\mathbf{a-b, b+c,} \\ -\mathbf{a+b-c} \\ (hex. axes) \\ \text{conjugate: } \mathbf{a+b, -b+c,} \\ \mathbf{a-b-c} \\ (hex. axes) \\ \text{conjugate: } -\mathbf{a+b, -b-c,} \\ -\mathbf{a-b+c} \\ (hex. axes) \\ \end{array}$	$\begin{array}{c} \frac{1}{3}(2x-y-z),\\ \frac{1}{3}(x+y-2z),\\ \frac{1}{3}(x+y+z)-\frac{1}{4}\\ \frac{1}{3}(-2x-y+z),\\ \frac{1}{3}(-x+y+2z),\\ \frac{1}{3}(-x+y-z)-\frac{1}{4}\\ \frac{1}{3}(2x+y+z),\\ \frac{1}{3}(x-y-2z),\\ \frac{1}{3}(x-y-z)-\frac{1}{4}\\ \frac{1}{3}(-2x+y-z),\\ \frac{1}{3}(-x-y-2z),\\ \frac{1}{3}(-x-y+z)-\frac{1}{4}\end{array}$	$\begin{array}{c} \frac{1}{3}(2x-y-z),\\ \frac{1}{3}(x+y-2z),\\ \frac{1}{3}(x+y+z)\\ \frac{1}{3}(-2x-y+z)+\frac{1}{2},\\ \frac{1}{3}(-x+y+2z)+\frac{1}{2},\\ \frac{1}{3}(-x+y-z)\\ \frac{1}{3}(2x+y+z),\\ \frac{1}{3}(x-y+2z)+\frac{1}{2},\\ \frac{1}{3}(x-y-z)\\ \frac{1}{3}(-2x+y-z)+\frac{1}{2},\\ \frac{1}{3}(-x-y-2z),\\ \frac{1}{3}(-x-y+z)\\ \frac{1}{3}(-x-y+z)\end{array}$	6 <i>a</i>	18e	6b;18d	36 <i>f</i> 2×36 <i>f</i>	36 <i>f</i> 2×18 <i>e</i> ;36 <i>f</i>	12 <i>c</i> ;36 <i>f</i> 4×36 <i>f</i>
[3] <i>P</i> 4/ <i>nnc</i> (126)			2 <i>a</i>	2 <i>b</i> ;4 <i>c</i>	8 <i>f</i>	4d;8j 8g;2 imes 8j	4e;8i 8h;16k	16 <i>k</i> 3×16 <i>k</i>
conjugate: <b>b</b> , <b>c</b> , <b>a</b> conjugate: <b>c</b> , <b>a</b> , <b>b</b>	<i>y</i> , <i>z</i> , <i>x</i> <i>z</i> , <i>x</i> , <i>y</i>	<i>y</i> , <i>z</i> , <i>x</i> <i>z</i> , <i>x</i> , <i>y</i>						

# II Maximal *klassengleiche* subgroups Enlarged unit cell, isomorphic

$[27]Pn\bar{3}n$	3 <b>a</b> , 3 <b>b</b> , 3 <b>c</b>	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z;$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z;$	2 <i>a</i> ;12 <i>e</i> ;16 <i>f</i> ;	6 <i>b</i> ;12 <i>e</i> ;24 <i>g</i> ;	8 <i>c</i> ;16 <i>f</i> ;	12 <i>d</i> ;24 <i>g</i> ;	3×12 <i>e</i> ;	$3 \times 16f;$
		$\underbrace{+(\frac{1}{2},0,0):+(0)}_{\pm(0,0):\pm(0,$	$(1, \frac{1}{2}, 0): \pm (0, 0, \frac{1}{2}):$	24h	24 <i>h</i> ;2×48 <i>i</i>	$4 \times 48i$	6×48 <i>i</i>	$6 \times 48i$	$8 \times 48i$
		$\pm (0, \frac{1}{3}, \frac{1}{3}); \pm (\frac{1}{3})$	(3,0) $(3,0)$ $(3,0$				$3 \times 24g;$	$3 \times 24h;$	27×48 <i>i</i>
		$\pm (0, \frac{1}{3}, \frac{2}{3}); \pm (\frac{1}{3})$	$(\frac{1}{3}, 0, \frac{2}{3}); \pm (\frac{1}{3}, \frac{2}{3}, 0);$				12×48 <i>i</i>	12×48 <i>i</i>	
		$ \begin{array}{c} \pm (\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \\ \pm (\frac{1}{3}, \frac{2}{3}, \frac{1}{3}) \end{array} $	); $\pm (\frac{1}{3}, \frac{1}{3}, \frac{2}{3})$ ; ); $\pm (\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$						
$[p^3]Pn\bar{3}n$	p <b>a</b> , p <b>b</b> , p <b>c</b>	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$	$2a; \frac{p-1}{2} \times 12e;$	$6b; \frac{p-1}{2} \times 12e;$	8 <i>c</i> ;	12 <i>d</i> ;	$p \times 12e;$	$p \times 16f;$
		$+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$\frac{p-1}{2} \times 16f$	$\frac{p-1}{2} \times 24g;$	$\frac{p-1}{2} \times 16f;$	$\frac{p-1}{2} \times 24g;$	$\frac{p(p^2-1)}{4} \times 48i$	$\frac{p(p^2-1)}{3} \times$
	p = prime >	$2; u, v, w = 1, \dots$	, p - 1	$\frac{p-1}{2} \times 24h;$	$\frac{p-1}{2} \times 24h;$	$\frac{p(p^2-1)}{6} \times 48i$	$\frac{p(p^2-1)}{4} \times 48i$		481
				$\frac{p^3-13p+12}{24}\times$	$\frac{p^3-5p+4}{8}$ × 48 <i>i</i>				
				401			$p \times 24g;$	$p \times 24h;$	$p^3 \times 48i$
							$\frac{p(p^2-1)}{2} \times 48i$	$\frac{p(p^2-1)}{2} \times 48i$	