

## 8.3. Special topics on space groups

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## 8.3.1. Coordinate systems in crystallography

The matrices  $W$  and the columns  $w$  of crystallographic symmetry operations  $W$  depend on the choice of the coordinate system. A suitable choice is essential if  $W$  and  $w$  are to be obtained in a convenient form.

## Example

In a space group  $I4mm$ , the matrix part of a clockwise fourfold rotation around the  $c$  axis is described by the  $W$  matrix

$$4^- 00z : \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

if referred to the *conventional* crystallographic basis  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ . Correspondingly, the matrix

$$m 0yz : \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

represents a reflection in a plane parallel to  $\mathbf{b}$  and  $\mathbf{c}$ . These matrices are easy to handle and their geometrical significance is evident. Referred to the *primitive* basis  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$ , defined by  $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$ ,  $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$ ,  $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ , the matrices representing the same symmetry operations would be

$$4^- : \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \end{pmatrix}; \quad m : \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}.$$

These matrices are more complicated to work with, and their geometrical significance is less obvious.

The conventional coordinate systems obey rules concerning the vector bases and the origins.

(i) In all cases, the *conventional* coordinate bases are chosen such that the matrices  $W$  only consist of the integers 0, +1 and -1, that they are reduced as much as possible, and that they are of simplest form, *i.e.* contain six or at least five zeros for three dimensions and two or at least one zeros for two dimensions. This fact can be expressed in geometric terms by stating that ‘symmetry directions (*Blickrichtungen*) are chosen as coordinate axes’ (axes of rotation, screw rotation or rotoinversion, normals of reflection or glide planes); *cf.* Section 2.2.4 and Chapter 9.1. Shortest translation vectors compatible with these conditions are chosen as basis vectors. In many cases, the conventional vector basis is not a primitive but rather a nonprimitive crystallographic basis, *i.e.* there are lattice vectors with fractional coefficients. The centring type of the conventional cell and thus the lattice type can be recognized from the first letter of the Hermann–Mauguin symbol.

## Example

The letter  $P$  for  $E^3$  (or  $p$  for  $E^2$ ), taken from ‘primitive’, indicates that a primitive basis is being used conventionally for describing the crystal structure and its symmetry operations. In this case, the vector lattice  $\mathbf{L}$  consists of all vectors  $\mathbf{u} = u_1\mathbf{a}_1 + \dots + u_n\mathbf{a}_n$  with integral coefficients  $u_i$ , but contains no other vectors. If the Hermann–Mauguin symbol starts with a ‘ $C$ ’ in  $E^3$  or with a ‘ $c$ ’ in  $E^2$ , in addition to all such vectors  $\mathbf{u}$  all vectors  $\mathbf{u} + \frac{1}{2}(\mathbf{a} + \mathbf{b})$  also belong to  $\mathbf{L}$ . The letters  $A$ ,  $B$ ,  $I$ ,  $F$  and  $R$  are used for the conventional bases of the other types of lattices, *cf.* Section 1.2.1.

In a number of cases, the symmetry of the space group determines the conventional vector basis uniquely; in other cases, metrical criteria, *e.g.* the length of basis vectors, may be used to define a conventional vector basis.

(ii) The choice of the *conventional origin* in the space-group tables of this volume has been dealt with by Burzlaff & Zimmermann (1980). In general, the origin is a point of highest site symmetry, *i.e.* as many symmetry operations  $W_j$  as possible leave the origin fixed, and thus have  $w_j = \mathbf{o}$ . Special reasons may justify exceptions from this rule, for example for space groups  $I2_12_12_1 \equiv D_2^9$  (No. 24),  $P4_332 \equiv O^6$  (No. 212),  $P4_132 \equiv O^7$  (No. 213),  $I4_132 \equiv O^8$  (No. 214) and  $I43d \equiv T_d^6$  (No. 220); *cf.* Section 2.2.7. If in a centrosymmetric space group a centre of inversion is not a point of highest site symmetry, the space group is described twice, first with the origin in a point of highest site symmetry, and second with the origin in a centre of inversion, *e.g.* at 222 and at  $\bar{1}$  for space group  $Pnmm \equiv D_{2h}^2$  (No. 48); *cf.* Section 2.2.1.\* For space groups with low site symmetries, the origin is chosen so as to minimize the number of nonzero coefficients of the  $w_j$ , *e.g.* on a twofold screw axis for space group  $P2_1 \equiv C_2^2$  (No. 4).

A change of the coordinate system, *i.e.* referring the crystal pattern and its symmetry operations  $W$  to a new coordinate system, results in new coordinates  $x'$  and new matrices  $W'$ ; *cf.* Section 5.1.3.

## 8.3.2. (Wyckoff) positions, site symmetries and crystallographic orbits

The concept of *positions* and their *site symmetries* is fundamental for the determination and description of crystal structures. Let, for instance,  $P\bar{1}$  be the space group of a crystal structure with tetrahedral  $AX_4$  and triangular  $BY_3$  groups. Then the atoms  $A$  and  $B$  cannot be located at centres of inversion, as the symmetry of tetrahedra and triangles is incompatible with site symmetry  $\bar{1}$ . If the space group is  $P2/m$ , again the points with site symmetry  $2/m$  cannot be the loci of  $A$  or  $B$ , but points with site symmetries  $2$ ,  $m$  or  $1$  can.

The relations between ‘site symmetry’ and ‘positions’ can be formulated in a rather general way.

*Definition:* The set of all symmetry operations of a space group  $\mathcal{G}$  that leave a point  $X$  invariant forms a finite group, the *site-symmetry group*  $\mathcal{S}(X)$  of  $X$  with respect to  $\mathcal{G}$ .†

With regard to the symmetry operations of a space group  $\mathcal{G}$ , two kinds of points are to be distinguished. A point  $X$  is called a *point of general position* with respect to a space group  $\mathcal{G}$  if there is no symmetry operation of  $\mathcal{G}$  (apart from the identity operation) that leaves  $X$  fixed, *i.e.* if  $\mathcal{S}(X) = \mathcal{I}$ . A point  $X$  is called a *point of special position* with respect to a space group  $\mathcal{G}$  if there is at least one other symmetry operation of  $\mathcal{G}$ , in addition to the identity operation, that leaves  $X$  fixed, *i.e.* if  $\mathcal{S}(X) > \mathcal{I}$ .

The subdivision of the set of all points into two classes, those of general and those of special position with respect to a space group

\* Also space group  $P4_2/nm \equiv D_{4h}^{16}$  (No. 138) is listed with two origins. The first origin is chosen at a point with site symmetry 4 as in Hermann (1935). The site symmetries ( $2/m$ ) of the centres of inversion have the same order 4.

† Instead of ‘site-symmetry group’, the term ‘point group’ is frequently used for the local symmetry in a crystal structure or for the symmetry of a molecule. In order to avoid confusion, in this chapter the term ‘point group’ is exclusively used for the symmetry of the external shape and of the physical properties of the macroscopic crystal, *i.e.* for a symmetry in vector space.

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$\mathcal{G}$ , constitutes only a very coarse classification. A finer classification is obtained as follows.

*Definition:* A Wyckoff position  $W_{\mathcal{G}}$  (for short, position; in German, *Punktlage*) consists of all points  $X$  for which the site-symmetry groups  $\mathcal{S}(X)$  are conjugate subgroups\* of  $\mathcal{G}$ .

For practical purposes, each Wyckoff position of a space group is labelled by a letter which is called the *Wyckoff letter* (*Wyckoff notation* in earlier editions of these *Tables*). Wyckoff positions *without* variable parameters (e.g.  $0, 0, 0; 0, 0, \frac{1}{2}; \dots$ ) and *with* variable parameters (e.g.  $x, y, z; x, 0, \frac{1}{4}; \dots$ ) have to be distinguished.

The number of different Wyckoff positions of each space group is finite, the maximal numbers being nine for plane groups (realized in  $p2mm$ ) and 27 for space groups (realized in  $Pmmm$ ).

A finer classification of the points of  $E^n$  with respect to  $\mathcal{G}$ , which always results in an infinite number of classes, is the subdivision of all points into sets of symmetrically equivalent points. In the following, these sets will be called crystallographic orbits according to the following definition.

*Definition:* The set of all points that are symmetrically equivalent to a point  $X$  with respect to a space group  $\mathcal{G}$  is called the *crystallographic orbit* of  $X$  with respect to  $\mathcal{G}$ .

#### Example

Described in a conventional coordinate system, the crystallographic orbit of a point  $X$  of general position with respect to a plane group  $p2$  consists of the points  $x, y; \bar{x}, \bar{y}; x + 1, y; \bar{x} + 1, \bar{y}; x, y + 1; \bar{x}, \bar{y} + 1; x - 1, y; \bar{x} - 1, \bar{y}; x, y - 1; \bar{x}, \bar{y} - 1; x + 1, y + 1; \dots$  etc.

Crystallographic orbits are infinite sets of points due to the infinite number of translations in each space group. Any one of its points may represent the whole crystallographic orbit, i.e. may be the generating point  $X$  of a crystallographic orbit.†

Because the site-symmetry groups of different points of the same crystallographic orbit are conjugate subgroups of  $\mathcal{G}$ , a crystallographic orbit consists either of points of general position or of points of special position only. Therefore, one can speak of ‘crystallographic orbits of general position’ or *general crystallographic orbits* and of ‘crystallographic orbits of special position’ or *special crystallographic orbits* with respect to  $\mathcal{G}$ . Because all points of a crystallographic orbit belong to the same Wyckoff position of  $\mathcal{G}$ , one also can speak of *Wyckoff positions of crystallographic orbits*.‡

The points of each *general crystallographic orbit* of a space group  $\mathcal{G}$  are in a one-to-one correspondence with the symmetry operations of  $\mathcal{G}$ . Starting with the generating point  $X$  (to which the identity operation corresponds), to each point  $\tilde{X}$  of the crystallographic orbit belongs exactly one symmetry operation  $W$  of  $\mathcal{G}$  such that  $\tilde{X}$  is the image of  $X$  under  $W$ . This one-to-one correspondence is the reason why the ‘coordinates’ listed for the general position in the space-group tables may be interpreted in two different ways, either as the coordinates of the image points of  $X$  under  $\mathcal{G}$  or as a short-hand notation for the pairs  $(W, w)$  of the symmetry operations  $W$  of  $\mathcal{G}$ ; cf. Sections 8.1.6 and 11.1.1. Such a

one-to-one correspondence does not exist for the *special crystallographic orbits*, where each point corresponds to a complete coset of a left coset decomposition of  $\mathcal{G}$  with respect to the site-symmetry group  $\mathcal{S}(X)$  of  $X$ . Thus, the data listed for the special positions are to be understood only as the coordinates of the image points of  $X$  under  $\mathcal{G}$ .

Space groups with no special crystallographic orbits are called *fixed-point-free space groups*. The following types of fixed-point-free space groups occur:  $p1$  and  $pg$  in  $E^2$ ;  $P_1 \equiv C_1^1$  (No. 1),  $P_2 \equiv C_2^2$  (No. 4),  $Pc \equiv C_s^2$  (No. 7),  $Cc \equiv C_s^4$  (No. 9),  $P_2 \equiv C_2^4$  (No. 19),  $Pca \equiv C_{2v}^5$  (No. 29),  $Pna \equiv C_{2v}^9$  (No. 33),  $P_4 \equiv C_4^2$  (No. 76),  $P_4 \equiv C_4^4$  (No. 78),  $P_3 \equiv C_3^2$  (No. 144),  $P_3 \equiv C_3^3$  (No. 145),  $P_6 \equiv C_6^2$  (No. 169) and  $P_6 \equiv C_6^3$  (No. 170) in  $E^3$ .

Though the classification of the points of space  $E^n$  into Wyckoff positions  $W_{\mathcal{G}}$  of a space group  $\mathcal{G}$  is unique, the labelling of the Wyckoff positions by Wyckoff letters (Wyckoff notation) is not.

#### Example

In a space group  $P\bar{1}$  there are eight classes of centres of inversion  $\bar{1}$ , represented in the space-group tables by  $0, 0, 0; 0, 0, \frac{1}{2}; 0, \frac{1}{2}, 0; \dots; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ . The site-symmetry groups  $\{1, \bar{1}\}$  within each class are ‘symmetrically equivalent’, i.e. they are conjugate subgroups of  $P\bar{1}$ . The groups  $\{1, \bar{1}\}$  of *different* classes, however, are *not* ‘symmetrically equivalent’ with respect to  $P\bar{1}$ . Each class is labelled by one of the Wyckoff letters  $a, b, \dots, h$ . This letter depends on the choice of origin and on the choice of coordinate axes. Cyclic permutation of the labels of the basis vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$ , for instance, induces a cyclic permutation of Wyckoff positions  $b-c-d$  and  $e-f-g$ ; origin shift from  $0, 0, 0$  to the point  $\frac{1}{2}, 0, 0$  results in an exchange of Wyckoff letters in the pairs  $a-d, b-f, c-e$  and  $g-h$ . Even if the coordinate axes are determined by some extra condition, e.g.  $a \leq b \leq c$ , there exist no rules for fixing the origin in  $P\bar{1}$  when describing a crystal structure. The eight classes of centres of inversion of  $P\bar{1}$  are well established but none of them is inherently distinguished from the others.

The example shows that the different Wyckoff positions of a space group  $\mathcal{G}$  may permute under an isomorphic mapping of  $\mathcal{G}$  onto itself, i.e. under an automorphism of  $\mathcal{G}$ . Accordingly, it is useful to collect into one set all those Wyckoff positions of a space group  $\mathcal{G}$  that may be permuted by automorphisms of  $\mathcal{G}$ . These sets are called ‘Wyckoff sets’. The Wyckoff letters belonging to the different Wyckoff positions of the same Wyckoff set are listed by Koch & Fischer (1975); changes in Wyckoff letters caused by changes of the coordinate system have been listed by Boyle & Lawrenson (1973, 1978).

To introduce ‘Wyckoff sets’ more formally, it is advantageous to use the concept of normalizers; cf. Ledermann (1976). The *affine normalizer*  $\mathcal{N}\S$  of a space group  $\mathcal{G}$  in the group  $\mathcal{A}$  of all affine mappings is the set of those affine mappings which map  $\mathcal{G}$  onto itself. The space group  $\mathcal{G}$  is a normal subgroup of  $\mathcal{N}$ ,  $\mathcal{N}$  itself is a subgroup of  $\mathcal{A}$ . The mappings of  $\mathcal{N}$  which are not symmetry operations of  $\mathcal{G}$  may transfer one Wyckoff position of  $\mathcal{G}$  onto another Wyckoff position.

*Definition:* Let  $\mathcal{N}$  be the normalizer of a space group  $\mathcal{G}$  in the group of all affine mappings. A *Wyckoff set* with respect to  $\mathcal{G}$  consists of all points  $X$  for which the site-symmetry groups are conjugate subgroups of  $\mathcal{N}$ .

The difference between Wyckoff positions and Wyckoff sets of  $\mathcal{G}$  may be explained as follows. Any Wyckoff position of  $\mathcal{G}$  is transformed onto itself by all elements of  $\mathcal{G}$ , but not necessarily by the elements of the (larger) group  $\mathcal{N}$ . Any Wyckoff set, however, is

\* For the term ‘conjugate subgroups’, see Section 8.3.6.

† For the crystallographic orbits different names have been used by different authors: *regelmässiges Punktsystem*, Sohncke (1879) and Schoenflies (1891); *regular system of points*, Fedorov (1891); *Punktkonfiguration*, Fischer & Koch (1974); *orbit*, Wondratschek (1976); *point configuration*, Fischer & Koch (1978) and Part 14 of this volume; *crystallographic orbit*, Matsumoto & Wondratschek (1979) and Wondratschek (1980).

‡ Fischer & Koch (1974) use the name *Punktlage*.

§ Section 8.3.6 and Part 15 deal with normalizers of space groups in more detail.

transformed onto itself even by those elements of  $\mathcal{N}$  which are not contained in  $\mathcal{G}$ .

*Remark:* A Wyckoff set of  $\mathcal{G}$  is a set of points. Obviously, with each point  $X$  it contains all points of the crystallographic orbit of  $X$  and all points of the Wyckoff position of  $X$ . Accordingly, one can speak not only of ‘Wyckoff sets of points’, but also of ‘Wyckoff sets of crystallographic orbits’ and ‘Wyckoff sets of Wyckoff positions’ of  $\mathcal{G}$ . Wyckoff sets of crystallographic orbits have been used in the definition of lattice complexes (*Gitterkomplexe*), under the name *Konfigurationslage*, by Fischer & Koch (1974); cf. Part 14.

The concepts ‘crystallographic orbit’, ‘Wyckoff position’ and ‘Wyckoff set’ have so far been defined for individual space groups only. It is no problem, but is of little practical interest, to transfer the concept of ‘crystallographic orbit’ to space-group types. It would be, on the other hand, of great interest to transfer ‘Wyckoff positions’ from individual space groups to space-group types. As mentioned above, however, such a step is not unique. For this reason, the concept of ‘Wyckoff set’ has been introduced to replace ‘Wyckoff positions’. Different space groups of the same space-group type have corresponding Wyckoff sets, and one can define ‘types of Wyckoff sets’ (consisting of individual Wyckoff sets) in the same way that ‘types of space groups’ (consisting of individual space groups) were defined in Section 8.2.2.

*Definition:* Let the space groups  $\mathcal{G}$  and  $\mathcal{G}'$  belong to the same space-group type. The Wyckoff sets  $K$  of  $\mathcal{G}$  and  $K'$  of  $\mathcal{G}'$  belong to the same *type of Wyckoff sets* if the affine mappings which transform  $\mathcal{G}$  onto  $\mathcal{G}'$  also transform  $K$  onto  $K'$ .

Types of Wyckoff sets have been used by Fischer & Koch (1974), under the name *Klasse von Konfigurationslagen*, when defining lattice complexes. There are 1128 types of Wyckoff sets of the 219 (affine) space-group types and 51 types of Wyckoff sets of the 17 plane-group types [Koch & Fischer (1975) and Chapter 14.1].

### 8.3.3. Subgroups and supergroups of space groups

Relations between crystal structures imply relations between their space groups, which can often be expressed by group–subgroup relations. These group–subgroup relations may be recognized from relations between the lattices and between the point groups of the crystal structures.

#### Example

The crystal structures of silicon, Si, and sphalerite, ZnS, belong to space-group types  $Fd\bar{3}m \equiv O_h^f$  (No. 227) and  $F43m \equiv T_d^2$  (No. 216) with lattice constants  $a_{\text{Si}} = 5.43$  and  $a_{\text{ZnS}} = 5.41$  Å. The structure of sphalerite is obtained from that of silicon by replacing alternately half of the Si atoms by Zn and half by S, and by adjusting the lattice constant. The strong connection between the two crystal structures is reflected in the relation between their space groups: the space group of sphalerite is a subgroup (of index 2) of that of silicon (ignoring the small difference in lattice constants).

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

#### Examples

NaCl and CaF<sub>2</sub> belong to the same space-group type  $Fm\bar{3}m \equiv O_h^f$  (No. 225) and have lattice constants  $a = 5.64$  and  $a = 5.46$  Å,

respectively. The ions, however, occupy unrelated positions and so the symmetry relation does not express a structural relation. Pyrite, FeS<sub>2</sub>, and solid carbon dioxide, CO<sub>2</sub>, belong to the same space-group type  $Pa\bar{3} \equiv T_h^6$  (No. 205). They have lattice constants  $a = 5.42$  and  $a = 5.55$  Å, respectively, and the particles occupy analogous Wyckoff positions. Nevertheless, the structures of these compounds are not related because the positional parameters  $x = 0.386$  of S in FeS<sub>2</sub> and  $x = 0.11$  of O in CO<sub>2</sub> differ so much that the coordinations of corresponding atoms are dissimilar.

To formulate group–subgroup relations some definitions are necessary:

*Definitions:* A set  $\{H_i\}$  of symmetry operations  $H_i$  of a space group  $\mathcal{G}$  is called a *subgroup*  $\mathcal{H}$  of  $\mathcal{G}$  if  $\{H_i\}$  obeys the group conditions, i.e. is a symmetry group. The subgroup  $\mathcal{H}$  is called a *proper subgroup* of  $\mathcal{G}$  if there are symmetry operations of  $\mathcal{G}$  not contained in  $\mathcal{H}$ . A subgroup  $\mathcal{H}$  of a space group  $\mathcal{G}$  is called a *maximal subgroup* of  $\mathcal{G}$  if there is no proper subgroup  $\mathcal{M}$  of  $\mathcal{G}$  such that  $\mathcal{H}$  is a proper subgroup of  $\mathcal{M}$ , i.e.  $\mathcal{G} > \mathcal{M} > \mathcal{H}$ .

*Examples:* Maximal subgroups  $\mathcal{H}$  of a space group  $P1$  with lattice vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  are, among others, subgroups  $P1$  for which  $\mathbf{a}'' = p\mathbf{a}, \mathbf{b}'' = \mathbf{b}, \mathbf{c}'' = \mathbf{c}, p$  prime. If  $p$  is not a prime number, e.g.  $p = q \cdot r$ , the subgroup  $\mathcal{H}$  is not maximal, because a proper subgroup  $\mathcal{M}$  exists with  $\mathbf{a}' = q\mathbf{a}, \mathbf{b}' = \mathbf{b}, \mathbf{c}' = \mathbf{c}$ .  $\mathcal{M}$  again has  $\mathcal{H}$  as a proper subgroup with  $\mathbf{a}'' = r\mathbf{a}', \mathbf{b}'' = \mathbf{b}', \mathbf{c}'' = \mathbf{c}'$ .

$P2_1/c$  has maximal subgroups  $P2_1, Pc$  and  $P\bar{1}$  with the same unit cell, whereas  $P1$  is obviously not a maximal subgroup of  $P2_1/c$ .

A three-dimensional space group may have subgroups with no translations (site-symmetry groups; cf. Section 8.3.2), with one- or two-dimensional lattices of translations (line groups, frieze groups, rod groups, plane groups and layer groups), or with a three-dimensional lattice of translations (space groups). The number of subgroups of a space group is always infinite.

In this section, only those subgroups of a space group will be considered which are also space groups. This includes all maximal subgroups because a maximal subgroup of a space group is itself a space group. To simplify the discussion, we suppose the set of all *maximal* subgroups of every space group to be known. In this case, any subgroup  $\mathcal{H}$  of a given space group  $\mathcal{G}$  may be obtained via a chain of maximal subgroups  $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_{r-1}, \mathcal{H}_r = \mathcal{H}$  such that  $\mathcal{G} = \mathcal{H}_0 > \mathcal{H}_1 > \mathcal{H}_2 > \dots > \mathcal{H}_{r-1} > \mathcal{H}_r = \mathcal{H}$  where  $\mathcal{H}_j$  is a maximal subgroup of  $\mathcal{H}_{j-1}$  of index  $[i_j]$ , with  $j = 1, \dots, r$ ; for the term ‘index’ see below and Section 8.1.6. There may be many such chains between  $\mathcal{G}$  and  $\mathcal{H}$ . On the other hand, all subgroups of  $\mathcal{G}$  of a given index  $[i]$  are obtained if all chains are constructed for which  $[i_1] * [i_2] * \dots * [i_r] = [i]$  holds.

For example,  $P2/c > P2 > P1, P2/c > P\bar{1} > P1, P2/c > Pc > P1$  are all possible chains of maximal subgroups for  $P2/c$  if the original translations are retained completely. The seven subgroups of index [4] with the same translations as the original space group  $P6_3/mcm$  are obtained via the 21 different chains of Fig. 8.3.3.1.

Not only the number of all subgroups but even the number of all maximal subgroups of a given space group is infinite. This infinite number, however, only occurs for a certain kind of subgroup and can be reduced as described below. It is thus useful to consider the different kinds of subgroups of a space group in a way introduced by Hermann (1929).

It should be kept in mind that all group–subgroup relations considered here are relations between individual space groups but they are valid for all space groups of a space-group type, as the following example shows. A particular space group  $P2$  has a subgroup  $P1$  which is obtained from  $P2$  by retaining all translations