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The Superspace Groups for Incommensurate Crystal Structures with a One-Dimensional Modulation

BY P. M. DE WOLFF

Vakgroep Fysische Kristallografie, Laboratory for Technical Physics, Technische Hogeschool, 2628 CJ Delft, The Netherlands

AND T. JANSSEN AND A. JANNER

Institute for Theoretical Physics, University of Nijmegen, 6525 ED Nijmegen, The Netherlands

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Abstract

A complete list of (3 + 1)-dimensional superspace groups is presented. These groups describe the symmetry of incommensurate crystal structures with a one-dimensional modulation. A short discussion is given of applications. Extinction rules and Bravais types are tabulated in order to facilitate the determination of the superspace-group symmetry.

1. Introduction

This paper deals with crystals giving sharp diffraction spots in a pattern which requires not three, but four, basis vectors in reciprocal space. Hence, a diffraction vector **H** can be written as

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}, \quad h, k, l, m \text{ integers}, \tag{1.1}$$

while the coefficients α, β and γ in

$$\mathbf{q} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^* \tag{1.2}$$

are not all fixed rational numbers. (The convention adopted here is $\mathbf{a}.\mathbf{a}^* = 1$ *etc.*)

Such crystals represent the case $d = 1$ among the larger set of 'incommensurate structures', requiring $3 + d$ reciprocal basis vectors, *cf.* Janner & Janssen (1977). The cases $d = 2$ and $d = 3$ are known to occur in nature as well, but they are less frequent than the case of 'one-dimensional modulation' ($d = 1$) considered here.

For these structures there is no three-dimensional space-group symmetry, but an extended symmetry concept, as explained below, restores the characteristic of crystals: a lattice of symmetry translations. In correspondence with (1.1), such a lattice requires four basis vectors. By setting **a***, **b*** and **c*** apart from **q** in (1.1), we imply that the lattice Λ^* spanned by these vectors is reciprocal to the 'basic lattice' Λ. The latter is chosen so as to express the periodicity of a relevant approximation to the real structure. Λ is determined to a large extent by the point symmetry of the diffraction spots in reciprocal space. If that diffraction aspect is *hexagonal*, *tetragonal*, *trigonal* or *orthorhombic*, all spots lie on an array of lines parallel to the main axis (for orthorhombic, one of the binary axes). In direct space, this corresponds to a two-dimensional net of symmetry translations in the usual sense. Hence, the incommensurability refers only to the sequence of spots on the lines just mentioned, the direction of which will be termed the **c*** direction throughout. The magnitude of **c*** (and thus of **c**) is not defined, though there are not more than two essentially different choices. For the *monoclinic* case: either there is an array as above ('axial monoclinic') or all spots lie in equidistant planes parallel to the mirror plane ('planar monoclinic'). In the latter case there is a true symmetry translation **c** along the binary axis. Though this leaves a much wider choice for the basic lattice than in the former case, there are again just two alternatives differing essentially from the symmetry point of view. If the diffraction aspect is *triclinic* there is not necessarily a concentration of spots. The basic lattice is not restricted geometrically but the symmetry is utterly trivial anyhow.

In any case the basic lattice is not completely determined by the geometry of the diffraction spots and a choice must be made. In that respect, two classes of structures can be distinguished.

(i) There is a conspicuous set of strong 'main reflections', situated on nodes of a lattice Λ^*, which can be made to correspond to $m = 0$ in (1.1). The vector **q** is essentially determined by the remaining reflections called satellites which have $m \neq 0$. Their intensity vanishes rapidly for increasing values of $|m|$. The basic lattice is clearly indicated as the one of which Λ^* forms the reciprocal lattice. The structure can be described by periodic distortions of a normal crystal structure, the so-called basic structure. This is the class studied by de Wolff (1974) [referred to as (I)].

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(ii) In reciprocal space, there is no unique lattice of striking main reflections accompanied by satellites. In the cases published so far, it has been found that the structures can be obtained again by periodic distortions, this time of a 'composite basic structure'. The latter consists of two or more interpenetrating normal crystal structures which are mutually incommensurate. Class (ii) was studied by Janner & Janssen (1980*b*) [indicated here as (II)].

Surprisingly, the symmetry of class (ii) structures can be described by exactly the same groups which express the symmetry of class (i) crystals. This can be understood by looking at Fig. 1, which illustrates the classes (i) and (ii) for the case of one-dimensional modulation of a one-dimensional crystal. Here we use the result (I) that, for $d = 1$, an incommensurate crystal in n-dimensional position space can be seen as the intersection of that space with an $(n + 1)$-dimensional crystal, the so-called supercrystal. Hence our incommensurate ($n = 1$) crystal appears on a line L intersecting a planar, two-dimensionally periodic structure. The crystal is incommensurate provided that L is not parallel to a net line of the planar translation net. The supercrystal consists of a pattern of lines with an oscillating density and/or direction but with a well-defined average direction. There is a distinct line for each atom of the crystal. The atomic positions coincide with the intersections of L with these lines.

In the class (i) structures, Fig. 1(*a*) and (*b*), these lines have just one average direction which is parallel to net lines of the translation net of the planar structure. Clearly the spacing between these net lines, measured on L, is the period of the one-dimensional basic lattice.

In the class (ii) structure of Fig. 1(*c*), however, the lines representing atoms have different average directions, each again parallel to a net line. The two corresponding net-line spacings, measured on L, are equally plausible periods for the basic lattice. From a structural standpoint, class (ii) may seem unacceptable since it leads to overlapping atoms in L. However, in higher dimensions ($n = 2$ or 3), it is easy to conceive of configurations free from overlap, as they do indeed occur for the compounds mentioned in (II) as well as for certain surface structures, *cf.* Janssen, Janner & de Wolff (1980).

The symmetry correspondence between the two classes can now be exemplified for linear crystals. As shown in (I), all symmetry operations of the planar structure which map the line L into a line parallel to it are relevant for the linear one. These are symmetry translations and, possibly, inversion. Hence structures in both classes can have a symmetry based on either $p1$ or $p\bar{1}$ for the planar supercrystal. Of course, less trivial and more numerous groups are involved in describing the symmetry of three-dimensional incommensurate crystals – but there, too, each can occur for structures in class (i) as well as in class (ii).

The present tabulation uses the basic lattice as a given reference system. It is therefore particularly suited to class (i) structures. On the other hand, it follows from the above conclusion that no possible symmetry group is excluded by our approach. Moreover, in all class (ii) structures we know at present, one of the

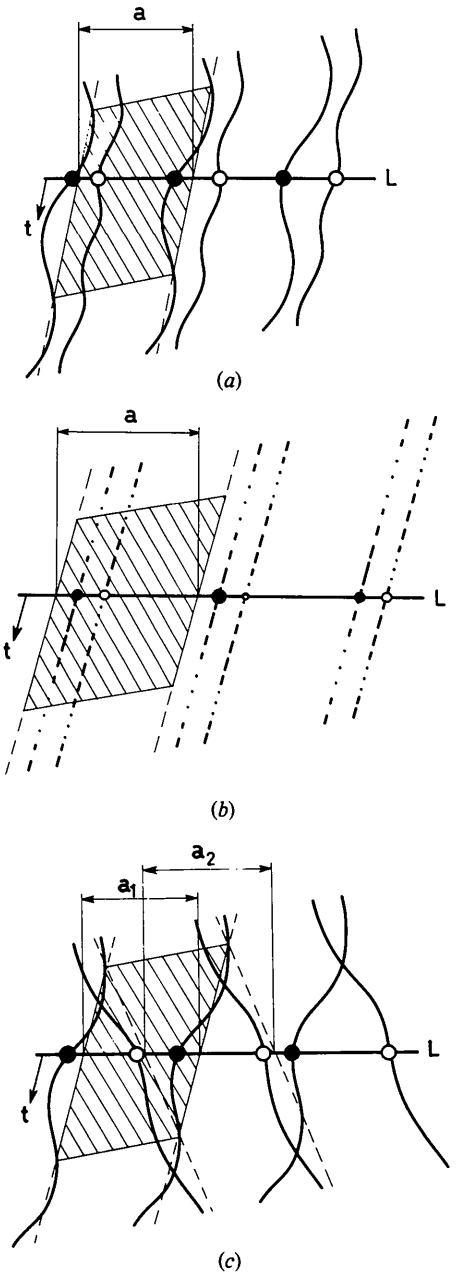

Fig. 1. Incommensurate one dimensional crystal structures with $d = 1$. For each case a unit cell of the two-dimensional supercrystal (shaded) and the period a of the basic lattice are shown. Atoms of two different kinds are indicated by full and open circles. (*a*) Class (i), displacive; (*b*) class (i), substitutional, as shown by varying dash length and circle size; (*c*) class (ii), displacive, with two equally plausible periods a_1 and a_2.

subsystems is distinguished as a host structure in the channels of which the other(s) are embedded. Then its basic lattice is the obvious choice for any description and is the best starting point for the classification here as well.

The basic lattice should not be associated too closely with the basic structure mentioned before. The latter is merely a zero-order approximation of the actual structure. It is not generally definable in an exact manner. A composite basic structure does not even possess a three-dimensional lattice of symmetry translations. In symmetry considerations the concept of a basic structure is not needed though it will be convenient to express symmetry operations in terms of such a concept.

2. Superspace groups

Symmetry operations can be described analytically (*cf.* § 3), but their principal features can be understood from Fig. 1. There we observe that any vector of the basic lattice in L becomes an extended symmetry translation vector if supplemented by a parallel shift of L, such that the resulting translation is a symmetry operation of the planar supercrystal. Similarly, if the supercrystal has inversion centres, each of these yields a symmetry operation on L provided that L is brought to the corresponding inverted position. In both cases, the supplementary operation (shift and/or inversion of the line L in the supercrystal) can be expressed as an operation on a coordinate t. This extra coordinate measures the position of L, from an arbitrary origin, in the direction of the net lines defining the basic lattice on L as discussed before. The t scale is determined by requiring that a shift $\Delta t = 1$ corresponds to a supercrystal period in the direction of those net lines (the t-axis direction).

The variable t expresses an extra degree of freedom, which can be visualized for class (i) crystals (especially displacive cases like those of Fig. 1*a*) as the movement of a wave through the crystal, but which is quite generally valid. In the case of d-dimensional modulation of a three-dimensional crystal, there are d extra degrees of freedom. They are comparable with the translational movements of a normal crystal in R_3. With these extra dimension(s), an appropriate new kind of symmetry operation (g_E, g_I) can be defined, where g_E is an element of a normal space group G_E in R_3 (the 'external' or 'positional' space) while g_I acts on d coordinates in the 'internal' space based on the extra dimension(s). The group G_E is called the *basic space group*. Often it is also the space group of the basic structure. The translations contained in G_E are those of the basic lattice.

The group formed by all operations (g_E, g_I) which leave the supercrystal, corresponding to an incommensurate structure, invariant will be called its superspace group. The appropriate form of g_E and g_I was worked out for the case $d = 1$ by de Wolff (1974, 1977), whereas Janner & Janssen (1977, 1979) have extended the theory to the general case. This work has been applied in various examples of symmetry classification by Bak & Janssen (1978) and Janner & Janssen (1980*a*,*b*). It has also led to several applications in structure analysis (van Aalst, Den Hollander, Peterse & de Wolff, 1976; Valentine, Cavin & Yakel, 1977; Yamamoto, Nakazawa & Tokonami, 1979) and to a theory on the dynamics of incommensurate crystals by Janssen (1979).

With a view to these and similar kinds of application, the authors have undertaken the derivation and complete listing of all superspace groups for the case $d = 1$. For two-dimensional incommensurate structures ($n = 2$), the relevant groups have been listed for both $d = 1$ and $d = 2$ by Janssen, Janner & de Wolff (1980). The list of Bravais types for $d = 1$ has been given by Janner, Janssen & de Wolff (1979).

A list of systematic extinctions is also given, so as to enable the user to identify the possible superspace group(s) for a given diffraction pattern.

The group tables follow the pattern of *International Tables for X-ray Crystallography* (1969). With the extended symbols, it should not be difficult to complete the g_E operations from those tables with the corresponding g_I ones in the form suited to the case at hand (that is, in terms of displacements, occupation densities or otherwise) by the rules given in §§ 3 and 4. Thus, a foundation is established for the calculation of structure factors or other structure-dependent quantities.

3. Symmetry operations

For incommensurate crystal structures with $d = 1$, locally defined quantities like the electron density ρ correspond to quantities $(\tilde{\rho})$ which do not merely depend on position $\mathbf{r}$ but also on t such that $\tilde{\rho}(\mathbf{r}, t = 0) = \rho(\mathbf{r})$. In the one-dimensional situation of Fig. 1, $\tilde{\rho}$ would correspond to a two-dimensional periodic function in the plane of that figure, while ρ is the value of that function on the line L (which corresponds to a constant value of t). A symmetry operation can be defined in terms of $\tilde{\rho}$ as follows. A combination of g_E: $\mathbf{r} \rightarrow \mathbf{r}'$ and g_I: $t \rightarrow t'$ is a symmetry operation if for all $\mathbf{r}, t$: $\tilde{\rho}(\mathbf{r}', t') = \tilde{\rho}(\mathbf{r}, t)$. It has the form

$$\mathbf{r}' = R\mathbf{r} + \mathbf{s} \tag{3.1}$$

$$t' = \varepsilon t + \delta - \mathbf{q}.\mathbf{s}. \tag{3.2}$$

(Another way of expressing a symmetry operation, in terms of, for example, atomic positions and displacements, is given in the second half of this section.) Here R, the homogeneous part of the normal space-group operation g_E, is a point-group operation; hence the

translation $\mathbf{s}$ can be split into an intrinsic part $\mathbf{s}_0$ and a part $\mathbf{s}_r$ which depends on the choice of origin:

$$\mathbf{s} = \mathbf{s}_0 + \mathbf{s}_r. \tag{3.3}$$

The intrinsic part, $\mathbf{s}_0$, is left invariant by R and is $1/n$ of the translation g_E^n when R is of order n. This part is non-zero only for translations ($R = 1$, $\mathbf{s}_0$ = translation vector) and for screw or glide operations. In (3.2), $\varepsilon = \pm 1$ and δ is a parameter which is an integer for all translations.

The combinations (R, ε) are restricted by the relation (de Wolff, 1977)

$$\varepsilon\mathbf{q} - R\mathbf{q} = \mathbf{n}^*, \tag{3.4}$$

where $\mathbf{n}^*$ is a vector of the reciprocal of the basic lattice. On the other hand, (3.4) is a restriction on $\mathbf{q}$ as well. This can be stated in terms of its (mutually perpendicular) components $\mathbf{q}_i$ and $\mathbf{q}_r$ such that

$$\mathbf{q} = \mathbf{q}_i + \mathbf{q}_r. \tag{3.5}$$

The vector $\mathbf{q}_i$ is the component of $\mathbf{q}$ in the subspace left invariant by εR for all pairs (R, ε) occurring in symmetry operations (3.1–3.2):

$$\varepsilon\mathbf{q}_i - R\mathbf{q}_i = 0. \tag{3.6}$$

For the systems yielding diffraction spots on lines or planes in reciprocal space (*cf. Introduction*), $\mathbf{q}_i$ is parallel to these lines or planes, while $\mathbf{q}_r$ is, if non-zero, normal to them. In the triclinic case, $\mathbf{q}_r = 0$. The coordinates of $\mathbf{q}_r$ (with respect to a basis of A^*) are simple rational fractions, whereas those of $\mathbf{q}_i$ are, in general, irrational.

In terms of the components of $\mathbf{s}$ and $\mathbf{q}$ introduced above, (3.2) becomes

$$t' = \varepsilon t + (\delta - \mathbf{q}_r.\mathbf{s}) - \mathbf{q}_i.\mathbf{s}_0 - \mathbf{q}_i.\mathbf{s}_r. \tag{3.7}$$

The last term $\mathbf{q}_i.\mathbf{s}_r$ is merely a correction needed if the origin is not situated on the symmetry element; it vanishes identically for $\varepsilon = +1$. The term $\mathbf{q}_i.\mathbf{s}_0$ is the intrinsic irrational change in t, since it is independent of the origin. Similarly, the term

$$\tau = \delta - \mathbf{q}_r.\mathbf{s} \tag{3.8}$$

can be called the intrinsic rational increment in t. This τ is invariant under a change of origin if $\varepsilon = +1$. (Strictly speaking for elements with $\varepsilon = -1$, τ is rational only for a suitable zero point on the t scale.) It is the most convenient parameter for characterizing g_I in superspace-group symbols as well as for extinctions.

The transformation of a distortion wave under the action of the superspace-group element (3.1–3.2) will now be described, firstly for the modulation of a scalar quantity. Consider a modulation of the occupation probability p_i for the ith atom ($i = 1, .., N$ if there are N atoms in the unit cell) of the basic structure. This function may, for example, describe the distribution of atoms over two different positions [see Janner & Janssen (1980*a*), § 7]. Such modulated quantities are periodic functions of $\mathbf{q}.\mathbf{r}_{ni}^0 + t$, where $\mathbf{r}_{ni}^0$ is the position of the ith atom in the unit cell given by the basic lattice vector $\mathbf{n}$. If $\mathbf{r}_i^0$ denotes its position within the unit cell, one has

$$\mathbf{r}_{ni}^0 = \mathbf{n} + \mathbf{r}_i^0. \tag{3.9}$$

The occupation probability for the atom in the position $\mathbf{r}_{ni}^0$ is

$$p = p_i(\mathbf{q}.\mathbf{r}_{ni}^0 + t). \tag{3.10}$$

The function $p_i(x)$ is periodic:

$$p_i(x + 1) = p_i(x). \tag{3.11}$$

If the operation (3.1) transforms the positions in such a way that

$$\mathbf{r}_{mj}^0 = R\mathbf{r}_{ni}^0 + \mathbf{s} \tag{3.12}$$

(where i and j denote atoms of the same chemical kind), the corresponding symmetry condition for p is

$$p_j(x) = p_i[\varepsilon(x - \delta + \mathbf{m}^*.\mathbf{r}_i^0)] \tag{3.13}$$

if the reciprocal-lattice vector $\mathbf{m}^*$ is given by $\mathbf{m}^* = \varepsilon\mathbf{q} - R^{-1}\mathbf{q}$.

The symmetry condition can also be formulated independently of the specific atom positions, but then one needs a cell-dependent function p_{ni} defined by

$$p_{ni}(\mathbf{q}_i.\mathbf{r}_{ni}^0 + t) = p_i(\mathbf{q}.\mathbf{r}_{ni}^0 + t). \tag{3.14}$$

Then (3.13) is equivalent to

$$p_{mj}(x) = p_{ni}[\varepsilon(x - \tau)]. \tag{3.15}$$

Similarly, the symmetry condition for a vector function, such as the displacement vector field $\mathbf{u}_i$ of the ith kind of atom in a displacively modulated crystal is

$$\mathbf{u}_j(x) = R\mathbf{u}_i[\varepsilon(x - \delta + \mathbf{m}^*.\mathbf{r}_i^0)]. \tag{3.16}$$

Now consider the case of composite crystals in class (ii), consisting of a number of interpenetrating mutually incommensurate subsystems like the iodine and TTF subsystems in TTF_7I_5 (Johnson & Watson 1976). The subsystems are labelled by the index ν. Each of them is supposed to be a somewhat distorted normal crystal structure, and is described with reference to the lattice of symmetry translations of its own basic structure with basis vectors $\mathbf{a}_{\nu 1}$, $\mathbf{a}_{\nu 2}$, $\mathbf{a}_{\nu 3}$. Usually, one of these lattices will serve as the basic lattice for the whole structure. Anyhow, the reciprocal-lattice vectors for each subsystem are possible diffraction vectors. This means that the reciprocal basis vectors of the νth subsystem can be expressed as in (1.1):

$$\mathbf{a}_{\nu k}^* = Z_{k1}^{\nu}\,\mathbf{a}^* + Z_{k2}^{\nu}\,\mathbf{b}^* + Z_{k3}^{\nu}\,\mathbf{c}^* + Z_{k4}^{\nu}\,\mathbf{q}, \quad k = 1, 2, 3, \tag{3.17}$$

Z_{ki}^{ν} being integer coefficients. Now the position of the ith atom ($i = 1, .., N_\nu$ if there are N_ν subsystem atoms in

their corresponding unit cell) in the unit cell $\mathbf{n}_\nu$ of the νth subsystem is given by

$$\mathbf{r}^0_{n\nu i} = \mathbf{n}_\nu + \mathbf{r}^0_{\nu i} - t \sum_{k=1}^{3} Z^\nu_{k4}\, \mathbf{a}_{\nu k}, \tag{3.18}$$

where $\{\mathbf{a}_{\nu k}\}$ $(k = 1, 2, 3)$ is the basis reciprocal to (3.17). So the positions depend linearly on t, except of course in the subsystem yielding the basic lattice ($Z^\nu_{k4} = 0$). If (3.1–3.2) is a symmetry transformation, then the position of the atom labelled by $n\nu i$ is transformed according to

$$\mathbf{r}^0_{m\mu j} = R(\mathbf{n}_\nu + \mathbf{r}^0_{\nu i}) + \mathbf{s} - \varepsilon(t - \delta + \mathbf{q}.\mathbf{s}) \sum_{k=1}^{3} Z^\nu_{k4}\, R\mathbf{a}_{\nu k}. \tag{3.19}$$

Conversely, if for every atom labelled by $n\nu i$ there is another one of the same chemical kind labelled by $m\mu j$, such that (3.19) holds, then the corresponding transformation (3.1–3.2) is a symmetry operation for the composite basic structure. (In the TTF_7I_5 example $\mu = \nu$, but this is not necessarily so.) In addition, there will, in general, exist an interaction between the subsystems leading to displacive modulation. For the ensuing displacements the transformation (3.16) is valid.

4. Bravais types, equivalence criteria and nomenclature

Since the transformations (3.1–3.2) define an operator in $(\mathbf{r}, t)$ space, superspace groups for $d = 1$ are in fact four-dimensional space groups. However, not every four-dimensional space group is a superspace group. The separation of each operation into g_E and g_I restricts the groups to the category of (3 + 1)-reducible groups. Further restrictions follow from relation (3.4).

The translations in R_4 are those transformations (3.1–3.2) for which $R = 1$. Hence, because $\mathbf{q}$ in (3.4) has at least one irrational component, $\varepsilon = 1$. They are given by

$$\mathbf{r}' = \mathbf{r} + \mathbf{n} \tag{4.1}$$

$$t' = t - \mathbf{q}.\mathbf{n} + m, \tag{4.2}$$

where $\mathbf{n}$ can be any vector of the basic lattice Λ and m any integer. Rather than using the Bravais types in R_4, we shall classify translation lattices for superspace groups by an equivalence principle adapted to the special rôle assigned to the basic lattice. Firstly, we call the *holohedral point group* of the lattice the group of all pairs (R, ε), with R an orthogonal transformation in R_3 and $\varepsilon = \pm 1$, such that the basic lattice Λ is left invariant by R and (R, ε) satisfies (3.4) for some $\mathbf{n}^*$ in the reciprocal lattice Λ^*. Then two incommensurate structures belong to the same *Bravais type* if there are bases of the basic lattices Λ and Λ' such that (i) the point groups consisting of elements R and R', respectively, have the same (matrix) form, (ii) for corresponding elements of the holohedral point groups, $\varepsilon = \varepsilon'$, (iii) the rational vectors $\mathbf{q}_r$ and $\mathbf{q}'_r$ have the same components, up to a common sign.

In this way, 24 Bravais types (or classes) are found. We denote them by the symbols of their superspace groups (see below). The full list given in Table 1 shows 14 types which are straightforward extensions of Bravais types in R_3. The remaining ten have various kinds of centring in planes or spaces containing the t axis. The latter are distinguished by their $\mathbf{q}_r$ vectors. For instance, if in (1.2) $\alpha = \frac{1}{2}$, $\beta = 0$ and γ is irrational (*i.e.* $\mathbf{q}_r = \frac{1}{2}\mathbf{a}^*$ and $\mathbf{q}_i$ is directed along $\mathbf{c}^*$), there is a symmetry

Table 1. *Reflection conditions for the 24 Bravais classes*

First column: number of the Bravais class. Second column: symbol of the Bravais class. Third column: relation between H, K, L in (5.1) and h, k, l in (1.1). If not stated otherwise: $H = h$, $K = k$, $L = l$. The axes transform as the indices when putting $m = 0$ in the third column. Fourth column: reflection conditions. Fifth column: $\mathbf{q}_i$ (top of each system) and $\mathbf{q}_r$ with respect to the conventional reciprocal basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$.

Triclinic				$\alpha\beta\gamma$
1	$P^{P\bar{1}}_{\bar{1}}$	–	–	000
Planar monoclinic (**c** unique)				$\alpha\beta 0$
2	$P^{P2/m}_{\bar{1}\,\bar{1}}$	–	–	000
3	$C^{P2/m}_{\bar{1}\,\bar{1}}$	$L = 2l + m$	$L + m = 2n$	$00\frac{1}{2}$
4	$P^{B2/m}_{\bar{1}\,\bar{1}}$	–	$H + L = 2n$	000
Axial monoclinic (**c** unique)				00γ
5	$P^{P2/m}_{1\,\bar{1}}$	–	–	000
6	$A^{P2/m}_{1\,\bar{1}}$	$H = 2h + m$	$H + m = 2n$	$\frac{1}{2}00$
7	$P^{B2/m}_{1\,\bar{1}}$	–	$H + L = 2n$	000
8	$B^{B2/m}_{1\,\bar{1}}$	$K = 2k + m$	$H + L = 2n, K + m = 2n'$	$0\frac{1}{2}0$
Orthorhombic				00γ
9	$P^{Pmmm}_{1\,1\,\bar{1}}$	–	–	000
10	$B^{Pmmm}_{1\,1\,\bar{1}}$	$K = 2k + m$	$K + m = 2n$	$0\frac{1}{2}0$
11	$W^{Pmmm}_{1\,1\,\bar{1}}$	$\begin{cases} K = 2k + m \\ H = 2h + m \end{cases}$	$K + m = 2n, H + m = 2n'$	$\frac{1}{22}0$
12	$P^{Immm}_{1\,1\,\bar{1}}$	–	$H + K + L = 2n$	000
13	$P^{Cmmm}_{1\,1\,\bar{1}}$	–	$H + K = 2n$	000
14	$L^{Cmmm}_{1\,1\,\bar{1}}$	$H = h + m$	$H + K + m = 2n$	100
15	$P^{Ammm}_{1\,1\,\bar{1}}$	–	$K + L = 2n$	000
16	$A^{Ammm}_{1\,1\,\bar{1}}$	$H = 2h + m$	$H + m = 2n, K + L = 2n'$	$\frac{1}{2}00$
17	$P^{Fmmm}_{1\,1\,\bar{1}}$	–	$H + K = 2n, H + L = 2n'$	000
18	$L^{Fmmm}_{1\,1\,\bar{1}}$	$H = h + m$	$H + K + m = 2n, K + L = 2n'$	100
Tetragonal				00γ
19	$P^{P4/mmm}_{1\,\bar{1}\,1\,1}$	–	–	000
20	$W^{P4/mmm}_{1\,\bar{1}\,1\,1}$	$\begin{cases} H = h + k + m \\ K = k - h \end{cases}$	$H + K + m = 2n$	$\frac{1}{22}0$
21	$P^{I4/mmm}_{1\,\bar{1}\,1\,1}$	–	$H + K + L = 2n$	000
Trigonal/hexagonal				00γ
22	$P^{R\bar{3}m}_{\bar{1}\,1}$	–	$H - K + L = 3n$	000
23	$R^{P\bar{3}1m}_{\bar{1}\,1\,1}$	$\begin{cases} H = 2h + k + m \\ K = k - h \end{cases}$	$H - K - m = 3n$	$\frac{1}{3}\frac{1}{3}0$
24	$P^{P6/mmm}_{1\,\bar{1}\,1\,1}$	–	–	000

translation which transforms coordinates according to (4.1–4.2) as $x \to x+1$, $y \to y$, $z \to z$, $t \to t-\frac{1}{2}$. So, in R_4, the x, t plane is centred. The lattice is a centring of the one with the same $\mathbf{q}_i$ but with $\mathbf{q}_r = 0$.

We define *superspace-group types* – that is, sets of equivalent superspace groups – by an equivalence principle, which is almost the same as for normal space groups. Two superspace groups are equivalent if there are right-handed bases in position space, a choice of origin in superspace and a choice of $\mathbf{q}$ (which is only determined up to a sign and up to a reciprocal-basic-lattice vector) such that (i) the matrices R, (ii) the elements ε, (iii) the components of $\mathbf{s}$, (iv) the values of τ (3.8) of G are the same as the corresponding ones for the elements of G'.

The equivalence principle being stronger than for space groups, nonequivalent superspace groups may be equivalent as four-dimensional space groups. This together with the fact that not all four-dimensional space groups may occur as superspace groups, is the reason why one cannot use here the list of four-dimensional space groups as given by Fast & Janssen (1968; only reducible ones) and by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978). The given equivalence principles are special cases of those given by Janner & Janssen (1979).

Superspace groups are denoted by a two-line symbol. The upper line contains the Hermann–Mauguin symbol for the basic space group. Below each generator g_E of this symbol the corresponding g_I is indicated by the intrinsic parameters in the following way. If $\varepsilon = -1$, there is always an origin such that τ vanishes. Then g_I is indicated by $\bar{1}$. If $\varepsilon = +1$ the value of τ is always one of the following:

$$\begin{array}{ll} \tau = & 0 \;\; \tfrac{1}{2} \;\; \pm\tfrac{1}{3} \;\; \pm\tfrac{1}{4} \;\; \pm\tfrac{1}{6} \\ \text{symbol} & 1 \;\; s \;\; t \;\; q \;\; h. \end{array} \tag{4.3}$$

The basic lattice type is determined by the basic space group, whereas zero components of the vector $\mathbf{q}_i$ follow from the group of pairs (R, ε). Since the superspace-group lattice is, according to (4.1–4.2), determined by Λ and $\mathbf{q}$, the only missing information is the vector $\mathbf{q}_r$. The symbol for this vector is a capital letter appearing as prefix to the Bravais-type symbol of the basic space group according to the following convention:

$$\begin{array}{lllllll} \mathbf{q}_r = & (000)_*, & (\tfrac{1}{2}00)_*, & (0\tfrac{1}{2}0)_*, & (00\tfrac{1}{2})_*, & (100)_*, & \\ \text{symbol} & P & A & B & C & L & \\ \mathbf{q}_r = & (010)_*, & (001)_*, & (0\tfrac{11}{22})_*, & (\tfrac{1}{2}0\tfrac{1}{2})_*, & (\tfrac{11}{22}0)_*, & (\tfrac{11}{33}0)_* \\ \text{symbol} & M & N & U & V & W & R \end{array} \tag{4.4}$$

As an example consider the group $L^{C2\frac{2}{1}mb}_{s1\bar{1}}$. The basic space group is $C2mb$. Choosing the origin as in *International Tables for X-ray Crystallography* (1969), m_y is associated with $\frac{1}{2}\mathbf{b}$. The (orthorhombic) space group has a lattice with conventional C-centred basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. A primitive basis is, for example, $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $-\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\mathbf{c}$. The vector $\mathbf{q}_i$ is along the $\mathbf{c}^*$ [because only in this direction is (3.6) satisfied] and $\mathbf{q}_r = (100)_*$ according to the prefix L. If we denote $\mathbf{r}$ by $x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = (x, y, z)$, the transforms of (x, y, z, t) under the four basic translations are

$$(x+\tfrac{1}{2}, y+\tfrac{1}{2}, z, t-\tfrac{1}{2}),\ (x-\tfrac{1}{2}, y+\tfrac{1}{2}, z, t+\tfrac{1}{2}),$$
$$(x, y, z+1, t-\gamma),\ (x, y, z, t+1). \tag{4.5}$$

The superspace-group symbol indicates that 2_x is combined with $\varepsilon = -1$ and m_y with $\varepsilon = +1$, $\tau = \frac{1}{2}$. Hence, the corresponding transforms of (x, y, z, t) are

$$(x, -y, -z, -t),\ (x, -y+\tfrac{1}{2}, z, t+\tfrac{1}{2}). \tag{4.6}$$

In Table 2, all superspace groups for three-dimensional incommensurate structures with $d = 1$ are given. The groups are arranged according to the sequence number of their basic space groups in *International Tables for X-ray Crystallography* (1969). The columns correspond to the Bravais types. In each row, the bottom line of the symbol is indicated by a number explained next to the symbol for the arithmetic crystal class. The superspace groups may be denoted either by the two-line symbol explained above or by a code consisting of three numbers: the first one is the number of the basic space group in *International Tables for X-ray Crystallography*, eventually with the addition of a letter to distinguish different settings; the second one is the number of the Bravais class (Table 1) and the third one indicates the bottom line as given in Table 2. As an example the group B^{Pma2}_{s1s} can also be denoted as $28a.10.2$.

5. Extinction rules

The diffraction vectors of a modulated crystal can be written as in (1.1). The basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ chosen there is not necessarily a primitive one. Satellites in one row or plane, as explained in § 1, are not assigned by (1.1) to the same main reflection if $\mathbf{q}_r \neq 0$. To avoid this it is convenient to choose another basis $\mathbf{a}_s$, $\mathbf{b}_s$, $\mathbf{c}_s$ in such a way that

$$\mathbf{H} = H\mathbf{a}_s^* + K\mathbf{b}_s^* + L\mathbf{c}_s^* + m\mathbf{q}_i, \quad H, K, L, m \text{ integers}, \tag{5.1}$$

which means that the components of $\mathbf{q}_r$ with respect to this basis are integers. The basis $\mathbf{a}_s^*$, $\mathbf{b}_s^*$, $\mathbf{c}_s^*$ can in most cases be obtained from $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ by halving one or two of the basis vectors. Only in two cases (one tetragonal, the other trigonal) are the axes also rotated.

On the other hand, one may express $\mathbf{H}$ always with respect to a primitive basis of Λ^*:

$$\mathbf{H} = n_1\,\mathbf{a}_1^* + n_2\,\mathbf{a}_2^* + n_3\,\mathbf{a}_3^* + m\,\mathbf{a}_4^*, \quad n_i \text{ integer}. \tag{5.2}$$

Table 2. *The superspace groups in* (3 + 1) *dimensions, describing incommensurate structures with a one-dimensional modulation*

The superspace groups are represented by digits arranged in columns. Above each column are given the Bravais class number (Table 1) and, as subheading, the arithmetic crystal class denoted by the symbol for its symmorphic superspace group. To the left of this, a legend relates the digit to the superspace group bottom line. Each line begins with the basic space group (symbol top line) with (underlined) its number in *International Tables for X-ray Crystallography* (1969). If a group occurs as basic space group in more than one line, an additional letter is used for distinction (*a*, *b*, *etc.*). A – sign in a column does not necessarily mean that the corresponding superspace group does not exist. It may be equivalent to a group mentioned elsewhere in the table. Example: with basic space group $Pc2m$, no. 28, and Bravais lattice type no. 10, the bottom lines 111 and $s1s$ occur for the setting (top line) $Pma2$, when $\mathbf{q}_i$ is parallel to the 2 axis. Bottom lines $1\bar{1}\bar{1}$ and $s\bar{1}\bar{1}$ occur for the setting $Pm2a$ ($\mathbf{q}_i$ normal to *a*). Bottom line $1\bar{1}\bar{1}$ only occurs for the setting $Pc2m$ ($\mathbf{q}_i$ normal to *m*). The superspace group numbers are, respectively, 28*a*.10.1/2, 28*b*.10.1/2 and 28*c*.10.1.

Triclinic

Bravais class	1
1:1	P^{P1}_{1}
1. $P1$	1
1:$\bar{1}$	$P^{P\bar{1}}_{\bar{1}}$
2. $P\bar{1}$	1

Monoclinic *P* (c unique)

Bravais class	2	3
1:$\bar{1}$	$P^{P2}_{\bar{1}}$	$C^{P2}_{\bar{1}}$
3*a*. $P2$	1	1
4*a*. $P2_1$	1	–
1:1 2:s	P^{Pm}_{1}	C^{Pm}_{1}
6*a*. Pm	12	1
7*a*. Pb	1	1
1:$\bar{1}$1 2:$\bar{1}$s	$P^{P2/m}_{\bar{1}\,1}$	$C^{P2/m}_{\bar{1}\,1}$
10*a*. $P2/m$	12	1
11*a*. $P2_1/m$	12	–
13*a*. $P2/b$	1	1
14*a*. $P2_1/b$	1	–

Bravais class	5	6
1:1 2:s	P^{PZ}_{1}	A^{P2}_{1}
3*b*. $P2$	12	1
4*b*. $P2_1$	1	1
1:$\bar{1}$	$P^{Pm}_{\bar{1}}$	$A^{Pm}_{\bar{1}}$
6b. Pm	1	1
7b. Pb	1	1

Bravais class	5	6
1:1$\bar{1}$ 2:s$\bar{1}$	$P^{P2/m}_{1\,\bar{1}}$	$A^{P2/m}_{1\,\bar{1}}$
10*b*. $P2/m$	12	1
11*b*. $P2_1/m$	1	1
13*b*. $P2/b$	12	1
14*b*. $P2_1/b$	1	1

Monoclinic *B* (c unique)

Bravais class	4
1:$\bar{1}$	$P^{B2}_{\bar{1}}$
5*a*. $B2$	1
1:1 2:s	P^{Bm}_{1}
8*a*. Bm	12
9*a*. Bb	1
1:$\bar{1}$1 2:$\bar{1}$s	$P^{B2/m}_{\bar{1}\,1}$
12*a*. $B2/m$	12
15*a*. $B2/b$	1

Bravais class	7	8
1:1 2:s	P^{B2}_{1}	B^{B2}_{1}
5*b*. $B2$	12	1
1:$\bar{1}$	$P^{Bm}_{\bar{1}}$	$B^{Bm}_{\bar{1}}$
8*b*. Bm	1	1
9*b*. Bb	1	–
1:1$\bar{1}$ 2:s$\bar{1}$	$P^{B2/m}_{1\,\bar{1}}$	$B^{2/m}_{1/\bar{1}}$
12*b*. $B2/m$	12	1
15*b*. $B2/b$	12	–

Orthorhombic *P*

Bravais class	9	10	11
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}$s	$P^{P222}_{\bar{1}\bar{1}1}$	$B^{P222}_{\bar{1}\bar{1}1}$	$W^{P222}_{\bar{1}\bar{1}1}$
16. $P222$	12	1	1
17*a*. $P222_1$	1	1	1
17*b*. $P2_122$	12	1	–
18*a*. $P2_12_12$	12	–	–
18*b*. $P2_122_1$	1	1	–
19. $P2_12_12_1$	1	–	–
1:111 2:s1s 3:ss1 4:1ss 5:qq1	P^{Pmm2}_{111}	B^{Pmm2}_{111}	W^{Pmm2}_{111}
25*a*. $Pmm2$	123	12	1
26*a*. $Pmc2_1$	12	12	1
26*b*. $Pcm2_1$	–	1	–
27*a*. $Pcc2$	12	1	1

Orthorhombic *P* (cont.)

Bravais class	9	10	11
28*a*. $Pma2$	1234	12	–
29*a*. $Pca2_1$	14	1	–
30*a*. $Pcn2$	12	1	–
31*a*. $Pmn2_1$	12	12	–
32*a*. $Pba2$	123	–	5
33*a*. $Pbn2_1$	12	–	5
34*a*. $Pnn2$	12	–	5
1:1$\bar{1}\bar{1}$ 2:s$\bar{1}\bar{1}$	$P^{Pm2m}_{1\bar{1}\bar{1}}$	$B^{Pm2m}_{1\bar{1}\bar{1}}$	$W^{Pm2m}_{1\bar{1}\bar{1}}$
25*b*. $Pm2m$	–	12	–
28*b*. $Pm2a$	–	12	–
28*c*. $Pc2m$	–	1	–
32*b*. $Pc2a$	–	1	–
1:$\bar{1}$1$\bar{1}$ 2:$\bar{1}$s$\bar{1}$ 3:$\bar{1}$q$\bar{1}$	$P^{P2mm}_{\bar{1}1\bar{1}}$	$B^{P2mm}_{\bar{1}1\bar{1}}$	$W^{P2mm}_{\bar{1}1\bar{1}}$
25*c*. $P2mm$	12	1	1
26*c*. $P2_1am$	12	1	–
26*d*. $P2_1ma$	12	1	–
27*b*. $P2aa$	12	1	–
28*d*. $P2cm$	1	1	1
28*e*. $P2mb$	12	–	–
29*b*. $P2_1ca$	1	1	–
29*c*. $P2_1ab$	12	–	–
30*b*. $P2na$	1	1	–
30*c*. $P2an$	12	–	3
31*b*. $P2_1nm$	1	1	–
31*c*. $P2_1mn$	12	–	–
32*c*. $P2cb$	1	–	–
33*b*. $P2_1nb$	1	–	–
33*c*. $P2_1cn$	1	–	–
34*b*. $P2nn$	1	–	3
1:11$\bar{1}$ 2:s1$\bar{1}$ 3:ss$\bar{1}$ 4:1s$\bar{1}$ 5:qq$\bar{1}$	$P^{Pmmm}_{11\bar{1}}$	$B^{Pmmm}_{11\bar{1}}$	$W^{Pmmm}_{11\bar{1}}$
47. $Pmmm$	123	12	1
48. $Pnnn$	12	–	5
49*a*. $Pccm$	12	1	1
49*b*. $Pmaa$	1234	12	–
50*a*. $Pban$	123	–	5
50*b*. $Pcna$	12	1	–
51*a*. $Pmma$	1234	12	–
51*b*. $Pmam$	1234	12	–
51*c*. $Pmcm$	12	12	–
51*d*. $Pcmm$	–	1	1
52*a*. $Pnna$	12	–	–
52*b*. $Pbnn$	12	–	5
52*c*. $Pcnn$	12	–	–
53*a*. $Pmna$	12	12	–
53*b*. $Pcnm$	12	1	–
53*c*. $Pbmn$	1234	–	–

Orthorhombic *P* (cont.)

Bravais class	9	10	11
54*a*. $Pcca$	12	1	–
54*b*. $Pcaa$	14	1	–
54*c*. $Pbab$	1234	–	–
55*a*. $Pbam$	123	–	–
55*b*. $Pcma$	14	1	–
56*a*. $Pccn$	12	–	–
56*b*. $Pbnb$	12	–	–
57*a*. $Pcam$	14	1	–
57*b*. $Pmca$	12	12	–
57*c*. $Pbma$	1234	–	–
58*a*. $Pnnm$	12	–	–
58*b*. $Pmnn$	12	–	–
59*a*. $Pmmn$	123	–	–
59*b*. $Pmnm$	12	12	–
60*a*. $Pbcn$	12	–	–
60*b*. $Pnca$	12	–	–
60*c*. $Pbna$	12	–	–
61. $Pbca$	12	–	–
62*a*. $Pnma$	14	–	–
62*b*. $Pbnm$	12	–	–
62*c*. $Pmcn$	12	–	–

Orthorhombic *I*

Bravais class	12
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}$s	$P^{I222}_{\bar{1}\bar{1}1}$
23. $I222$	12
24. $I2_12_12_1$	1
1:111 2:s1s 3:ss1 4:1s1	P^{Imm2}_{111}
44*a*. $Imm2$	123
45*a*. $Iba2$	123
46*a*. $Ima2$	1234
1:1$\bar{1}$1 2:s$\bar{1}$s	$P^{I2mm}_{1\bar{1}1}$
44*b*. $I2mm$	12
45*b*. $I2cb$	1
46*b*. $I2mb$	12
46*c*. $I2cm$	1
1:11$\bar{1}$ 2:s1$\bar{1}$ 3:ss$\bar{1}$ 4:1s$\bar{1}$	$P^{Immm}_{11\bar{1}}$
71. $Immm$	123
72*a*. $Ibam$	123
72*b*. $Imcb$	1234
73. $Ibca$	123
74*a*. $Imma$	123
74*b*. $Icmm$	1234

Table 2 (*cont.*)

Orthorhombic *F*

Bravais class	17	18
1:$\bar{1}\bar{1}1$ 2:$\bar{1}\bar{1}s$	$P^{F222}_{\bar{1}\bar{1}1}$	$L^{F222}_{\bar{1}\bar{1}1}$
22. *F222*	12	1
1:111 2:*s*1*s* 3:*ss*1	P^{Fmm2}_{111}	L^{Fmm2}_{111}
42*a*. *Fmm2*	123	123
43*a*. *Fdd2*	123	–
1:$\bar{1}$1$\bar{1}$ 1:$\bar{1}s\bar{1}$	$P^{F2mm}_{\bar{1}1\bar{1}}$	$L^{F2mm}_{\bar{1}1\bar{1}}$
42*b*. *F2mm*	12	12
43*b*. *F2dd*	12	–
1:11$\bar{1}$ 2:*s*1$\bar{1}$ 3:*ss*$\bar{1}$	$P^{Fmmm}_{11\bar{1}}$	$L^{Fmmm}_{11\bar{1}}$
69. *Fmmm*	123	123
70. *Fddd*	123	–

Orthorhombic *C*

Bravais class	13	14
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}s$	$P^{C222}_{\bar{1}\bar{1}1}$	$L^{C222}_{\bar{1}\bar{1}1}$
20*a*. $C222_1$	1	1
21*a*. *C222*	12	12
1:111 2:*s*1*s* 3:*ss*1	P^{Cmm2}_{111}	L^{Cmm2}_{111}
35*a*. *Cmm2*	123	123
36*a*. $Cmc2_1$	12	12
37*a*. *Ccc2*	12	12
1:$\bar{1}$1$\bar{1}$ 2:$\bar{1}s\bar{1}$	$P^{C2mm}_{\bar{1}1\bar{1}}$	$L^{C2mm}_{\bar{1}1\bar{1}}$
38*a*. *C2mm*	12	12
39*a*. *C2mb*	12	12
40*a*. *C2cm*	1	1
41*a*. *C2cb*	1	1
1:11$\bar{1}$ 2:*s*1$\bar{1}$ 3:*ss*$\bar{1}$	$P^{Cmmm}_{11\bar{1}}$	$L^{Cmmm}_{11\bar{1}}$
63*a*. *Cmcm*	12	12
64*a*. *Cmca*	12	12
65*a*. *Cmmm*	123	123
66*a*. *Cccm*	12	12
67*a*. *Cmma*	12	12
68*a*. *Ccca*	12	12

Orthorhombic *A*

Bravais class	15	16
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}s$	$P^{A222}_{\bar{1}\bar{1}1}$	$A^{A222}_{\bar{1}\bar{1}1}$
20*b*. $A2_122$	12	–
21*b*. *A222*	12	1

Orthorhombic *A* (cont.)

Bravais class	15	16
1:$\bar{1}$1$\bar{1}$ 2:$\bar{1}s\bar{1}$	$P^{A2mm}_{\bar{1}1\bar{1}}$	$A^{A2mm}_{\bar{1}1\bar{1}}$
35*b*. *A2mm*	12	12
36*b*. $A2_1am$	12	–
36*c*. $A2_1ma$	12	–
37*b*. *A2aa*	12	–
1:111 2:*s*1*s* 3:*ss*1 4:1*ss*	P^{Amm2}_{111}	A^{Amm2}_{111}
38*b*. *Amm2*	1234	14
39*b*. *Abm2*	1234	14
40*b*. *Ama2*	1234	–
41*b*. *Aba2*	1234	–
1:$\bar{1}\bar{1}\bar{1}$ 2:*s*$\bar{1}\bar{1}$	$P^{Am2m}_{1\bar{1}\bar{1}}$	$A^{Am2m}_{1\bar{1}\bar{1}}$
38*c*. *Am2m*	12	1
39*c*. *Ac2m*	12	1
40*c*. *Am2a*	12	–
41*c*. *Ac2a*	12	–
1:11$\bar{1}$ 2:*s*1$\bar{1}$ 3:*ss*$\bar{1}$ 4:1*s*$\bar{1}$	$P^{Ammm}_{11\bar{1}}$	$A^{Ammm}_{11\bar{1}}$
63*b*. *Amam*	1234	–
63*c*. *Amma*	1234	–
64*b*. *Abma*	1234	–
64*c*. *Acam*	1234	–
65*b*. *Ammm*	1234	14
66*b*. *Amaa*	1234	–
67*b*. *Acmm*	1234	14
68*b*. *Acaa*	1234	–

Tetragonal *P*

Bravais class	19	20
1:1 2:*q* 3:*s*	P^{P4}_{1}	W^{P4}_{1}
75. *P4*	123	12
76. $P4_1$	1	1
77. $P4_2$	12	12
78. $P4_3$	1	1
1:$\bar{1}$	$P^{P\bar{4}}_{\bar{1}}$	$W^{P\bar{4}}_{\bar{1}}$
81. $P\bar{4}$	1	1
1:1$\bar{1}$ 2:*s*$\bar{1}$ 3:*q*$\bar{1}$	$P^{P4/m}_{1\bar{1}}$	$W^{P4/m}_{1\bar{1}}$
83. *P4/m*	12	1
84. $P4_2/m$	1	1
85. *P4/n*	12	3
86. $P4_2/n$	1	3
1:1$\bar{1}\bar{1}$ 2:*q*1$\bar{1}$ 3:*s*1$\bar{1}$	$P^{P422}_{1\bar{1}\bar{1}}$	$W^{P422}_{1\bar{1}\bar{1}}$
89. *P422*	123	12
90. $P42_12$	123	–
91. $P4_122$	1	1
92. $P4_12_12$	1	–

Tetragonal *P* (cont.)

Bravais class	19	20
93. $P4_222$	12	12
94. $P4_22_12$	12	–
95. $P4_322$	1	1
96. $P4_32_12$	1	–
1:111 2:*ss*1 3:1*ss* 4:*s*1*s* 5:*qq*1 6:*qqs*	P^{P4mm}_{111}	W^{P4mm}_{111}
99. *P4mm*	1234	13
100. *P4bm*	1234	56
101. $P4_2cm$	13	13
102. $P4_2nm$	13	56
103. *P4cc*	12	1
104. *P4nc*	12	5
105. $P4_2mc$	12	1
106. $P4_2bc$	12	5
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}s$	$P^{P\bar{4}2m}_{\bar{1}\bar{1}1}$	$W^{P\bar{4}2m}_{\bar{1}\bar{1}1}$
111. $P\bar{4}2m$	12	12
112. $P\bar{4}2c$	1	1
113. $P\bar{4}2_1m$	12	–
114. $P\bar{4}2_1c$	1	–
1:$\bar{1}$1$\bar{1}$ 2:$\bar{1}s\bar{1}$	$P^{P\bar{4}m2}_{\bar{1}1\bar{1}}$	$W^{P\bar{4}m2}_{\bar{1}1\bar{1}}$
115. $P\bar{4}m2$	12	1
116. $P\bar{4}c2$	1	1
117. $P\bar{4}b2$	12	1
118. $P\bar{4}n2$	1	1
1:1 $\bar{1}$11 2:*s* $\bar{1}$*s*1 3:1 $\bar{1}$ *ss* 4:*s* $\bar{1}$1*s* 5:*q* $\bar{1}$*q*1 6:*q* $\bar{1}$*qs*	$P^{P4/mmm}_{1\bar{1}11}$	$W^{P4/mmm}_{1\bar{1}11}$
123. *P4/mmm*	1234	13
124. *P4/mcc*	12	1
125. *P4/nbm*	1234	56
126. *P4/nnc*	12	5
127. *P4/mbm*	1234	–
128. *P4/mnc*	12	–
129. *P4/nmm*	1234	–
130. *P4/ncc*	12	–
131. $P4_2/mmc$	12	1
132. $P4_2/mcm$	13	13
133. $P4_2/nbc$	12	5
134. $P4_2/nnm$	13	56
135. $P4_2/mbc$	12	–
136. $P4_2/mnm$	13	–
137. $P4_2/nmc$	12	–
138. $P4_2/ncm$	13	–

Tetragonal *I*

Bravais class	21
1:1 2:*q* 3:*s*	P^{I4}_{1}
79. *I4*	123
80. $I4_1$	12
1:$\bar{1}$	$P^{I\bar{4}}_{\bar{1}}$

Tetragonal *I* (cont.)

Bravais class	21
82. $I\bar{4}$	1
1:1$\bar{1}$ 2:*s*$\bar{1}$	$P^{I4/m}_{1\bar{1}}$
87. *I4/m*	12
88. *I4/a*	1
1:1$\bar{1}\bar{1}$ 2:*q*1$\bar{1}$ 3:*s*1$\bar{1}$	$P^{I422}_{1\bar{1}\bar{1}}$
97. *I422*	123
98. $I4_122$	12
1:111 2:*ss*1 3:1*ss* 4:*s*1*s*	P^{I4mm}_{111}
107. *I4mm*	1234
108. *I4cm*	1234
109. $I4_1md$	12
110. $I4_1cd$	12
1:1$\bar{1}$1 2:*s*$\bar{1}$*s*1	$P^{I\bar{4}m2}_{1\bar{1}1}$
119. $I\bar{4}m2$	12
120. $I\bar{4}c2$	1
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}s$	$P^{I\bar{4}2m}_{\bar{1}\bar{1}1}$
121. $I\bar{4}2m$	12
122. $I\bar{4}2d$	1
1:1 $\bar{1}$11 2:*s* $\bar{1}$*s*1 3:1 $\bar{1}$*ss* 4:*s* $\bar{1}$1*s*	$P^{I4/mmm}_{1\bar{1}11}$
139. *I4/mmm*	1234
140. *I4/mcm*	1234
141. $I4_1/amd$	12
142. $I4_1/acd$	12

Trigonal *R*

Bravais class	22
1:1 2:*t*	P^{R3}_{1}
146. *R3*	12
1:$\bar{1}$	$P^{R\bar{3}}_{\bar{1}}$
148. $R\bar{3}$	1
1:1$\bar{1}$ 2:*t*$\bar{1}$	$P^{R32}_{1\bar{1}}$
155. *R32*	12
1:11 2:1*s*	P^{R3m}_{11}
160. *R3m*	12
161. *R3c*	1
1:$\bar{1}$1 2:$\bar{1}s$	$P^{R\bar{3}m}_{\bar{1}1}$

Table 2 (*cont.*)

Trigonal *R* (cont.)

Bravais class	22
166. $R\bar{3}m$	12
167. $R\bar{3}c$	1

Trigonal *P*

Bravais class	23	24
1:1 2:*t*	R^{P3}_{1}	P^{P3}_{1}
143. *P*3	1	12
144. $P3_1$	1	1
145. $P3_2$	1	1
1:$\bar{1}$	$R^{P\bar{3}}_{\bar{1}}$	$P^{P\bar{3}}_{\bar{1}}$
147. $P\bar{3}$	1	1
1:11$\bar{1}$ 2:*t*1$\bar{1}$	$R^{P312}_{11\bar{1}}$	$P^{P312}_{11\bar{1}}$
149. *P*312	1	12
151. $P3_112$	1	1
153. $P3_212$	1	1
1:1$\bar{1}$1 2:*t*$\bar{1}$1	$R^{P321}_{1\bar{1}1}$	$P^{P321}_{1\bar{1}1}$
150. *P*321	–	12
152. $P3_121$	–	1
154. $P3_221$	–	1

Trigonal *P* (cont.)

Bravais class	23	24
1:111 2:1*s*1	R^{P3m1}_{111}	P^{P3m1}_{111}
156. *P*3*m*1	–	12
158. *P*3*c*1	–	1
1:111 2:11*s*	R^{P31m}_{111}	P^{P31m}_{111}
157. *P*31*m*	12	12
159. *P*31*c*	1	1
1:$\bar{1}$11 2:$\bar{1}$1*s*	$R^{P\bar{3}1m}_{\bar{1}11}$	$P^{P\bar{3}1m}_{\bar{1}11}$
162. $P\bar{3}1m$	12	12
163. $P\bar{3}1c$	1	1
1:$\bar{1}$11 2:$\bar{1}$*s*1	$R^{P\bar{3}m1}_{\bar{1}11}$	$P^{P\bar{3}m1}_{\bar{1}11}$
164. $P\bar{3}m1$	–	12
165. $P\bar{3}c1$	–	1

Hexagonal *P*

Bravais class	24
1:1 2:*h* 3:*t* 4:*s*	P^{P6}_{1}

Hexagonal *P* (cont.)

Bravais class	24
168. *P*6	1234
169. $P6_1$	1
170. $P6_5$	1
171. $P6_2$	12
172. $P6_4$	12
173. $P6_3$	12
1:$\bar{1}$	$P^{P\bar{6}}_{\bar{1}}$
174. $P\bar{6}$	1
1:1$\bar{1}$ 2:*s*$\bar{1}$	$P^{P6/m}_{1\bar{1}}$
175. *P*6/*m*	12
176. $P6_3/m$	1
1:1$\bar{1}\bar{1}$ 2:*h*$\bar{1}\bar{1}$ 3:*t*$\bar{1}\bar{1}$ 4:*s*$\bar{1}\bar{1}$	$P^{P622}_{1\bar{1}\bar{1}}$
177. *P*622	1234
178. $P6_122$	1
179. $P6_522$	1
180. $P6_222$	12
181. $P6_422$	12
182. $P6_322$	12
1:111 2:*ss*1	P^{P6mm}_{111}

Hexagonal *P* (cont.)

Bravais class	24
3:1*ss* 4:*s*1*s*	
183. *P*6*mm*	1234
184. *P*6*cc*	14
185. $P6_3cm$	13
186. $P6_3mc$	13
1:$\bar{1}$1$\bar{1}$ 2:$\bar{1}$*s*$\bar{1}$	$P^{P\bar{6}m2}_{\bar{1}1\bar{1}}$
187. $P\bar{6}m2$	12
188. $P\bar{6}c2$	1
1:$\bar{1}\bar{1}$1 2:$\bar{1}\bar{1}$*s*	$P^{P\bar{6}2m}_{\bar{1}\bar{1}1}$
189. $P\bar{6}2m$	12
190. $P\bar{6}2c$	1
1:1 $\bar{1}$11 2:*s* $\bar{1}$*s*1 3:1 $\bar{1}$*ss* 4:*s* $\bar{1}$1*s*	$P^{P6/mmm}_{1\bar{1}11}$
191. *P*6/*mmm*	1234
192. *P*6/*mcc*	14
193. $P6_3/mcm$	13
194. $P6_3/mmc$	13

The basis $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ may be expressed in the basis $\mathbf{a}_s$, $\mathbf{b}_s$, $\mathbf{c}_s$ as follows:

$$\begin{aligned}\mathbf{a}_1 &= S_{11}\,\mathbf{a}_s + S_{21}\,\mathbf{b}_s + S_{31}\,\mathbf{c}_s\\ \mathbf{a}_2 &= S_{12}\,\mathbf{a}_s + S_{22}\,\mathbf{b}_s + S_{32}\,\mathbf{c}_s\\ \mathbf{a}_3 &= S_{13}\,\mathbf{a}_s + S_{23}\,\mathbf{b}_s + S_{33}\,\mathbf{c}_s.\end{aligned} \tag{5.3}$$

Then one can write the integer coefficients n_i in terms of H, K, L, m. This puts restrictions on the indices H, K, L, m which depend on the Bravais class. Conversely, the Bravais class may be determined from systematic extinctions among the indices.

As an example, we consider the Bravais class $L^{Fmmm}_{11\bar{1}}$. Then $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ span an orthogonal lattice and $\mathbf{q}_r = (100)_*$ has already integer components. Hence, $\{\mathbf{a}_s, \mathbf{b}_s, \mathbf{c}_s\}$ is the same as $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$, which is related to a primitive basis *via* the matrix

$$S = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \tag{5.4}$$

Comparing (5.1) with (1.1), one gets the relations

$$H = h + m, \quad K = k, \quad L = l. \tag{5.5}$$

Moreover, the centring matrix S (5.4) gives the relation with the n_i's. Hence,

$$n_1 = \frac{K+L}{2}, \quad n_2 = \frac{H+L-m}{2},$$

$$n_3 = \frac{H+K-m}{2}. \tag{5.6}$$

These are integers if and only if

$$K + L = 2n, \quad H + L + m = 2n' \quad (n, n' \text{ integers}). \tag{5.7}$$

On the other hand, if the spots can be described by (5.1) with $\mathbf{a}_s^*$, $\mathbf{b}_s^*$, $\mathbf{c}_s^*$ an orthogonal basis, with $\mathbf{q}_i = \gamma\mathbf{c}^*$ and such that (5.7) is satisfied, then one may conclude that the modulated crystal belongs to the Bravais class $L^{Fmmm}_{11\bar{1}}$. As a second example, consider the Bravais class $W^{P4/mmm}_{1\bar{1}11}$. Here $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ span a tetragonal lattice and $\mathbf{q}_r = (\frac{1}{2}\frac{1}{2}0)_*$. The vectors $\mathbf{H}$ are in the form (5.1) if one introduces the tetragonal basis $\mathbf{a}_s = \mathbf{a} + \mathbf{b}$, $\mathbf{b}_s = \mathbf{b} - \mathbf{a}$, $\mathbf{c}_s = \mathbf{c}$. Then

$$n_1 = \frac{H-K-m}{2}, \quad n_2 = \frac{H+K-m}{2},$$

$$n_3 = L. \tag{5.8}$$

Table 3. *Special conditions due to the translation parts of symmetry operations*

First column: reflections to which the conditions apply and orientation of the symmetry element. Second column: conditions and the corresponding symmetry operation. For the classes 11, 20 and 23 the deviating conditions are given as footnotes to the Table. Just as in Table 1, the conventional basis is chosen for **a**, **b**, **c**.

Planar monoclinic (**c** unique)								
$00L0$	**c**	$L=2n$:	$\left(\begin{smallmatrix}2_1\\\bar{1}\end{smallmatrix}\right)$					
$HK0m$	**c**	$K=2n$:	$\left(\begin{smallmatrix}b\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$			
Axial monoclinic/orthorhombic/tetragonal ($\mathbf{q}_i$ along **c**)								
$00Lm$	**c**	$L=2n$	$\left(\begin{smallmatrix}2_1\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}2\\s\end{smallmatrix}\right)$	$L+m=2n$:	$\left(\begin{smallmatrix}2_1\\s\end{smallmatrix}\right)$	
$H000$	**a**	$H=2n$:	$\left(\begin{smallmatrix}2_1\\\bar{1}\end{smallmatrix}\right)$					
$HK00$	**c**†	$H=2n$:	$\left(\begin{smallmatrix}a\\\bar{1}\end{smallmatrix}\right)$	$K=2n$:	$\left(\begin{smallmatrix}b\\\bar{1}\end{smallmatrix}\right)$	$H+K=2n$:	$\left(\begin{smallmatrix}n\\\bar{1}\end{smallmatrix}\right)$	
						$H+K=4n$:	$\left(\begin{smallmatrix}d\\\bar{1}\end{smallmatrix}\right)$	
$0KLm$	**a**†‡	$K=2n$:	$\left(\begin{smallmatrix}b\\1\end{smallmatrix}\right)$	$K+L=2n$:	$\left(\begin{smallmatrix}n\\1\end{smallmatrix}\right)$	$K+L+m=2n$:	$\left(\begin{smallmatrix}n\\s\end{smallmatrix}\right)$	
		$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$K+m=2n$:	$\left(\begin{smallmatrix}b\\s\end{smallmatrix}\right)$	$K+L=4n$:	$\left(\begin{smallmatrix}d\\1\end{smallmatrix}\right)$	
		$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$	$L+m=2n$:	$\left(\begin{smallmatrix}c\\s\end{smallmatrix}\right)$	$K+L+2m=4n$:	$\left(\begin{smallmatrix}d\\s\end{smallmatrix}\right)$	
Tetragonal								
$00Lm$	**c**	$L=2n$:	$\left(\begin{smallmatrix}4_2\\1\end{smallmatrix}\right)$	$L=4n$:	$\left(\begin{smallmatrix}4_1\\1\end{smallmatrix}\right)$	$2L+m=4n$:	$\left(\begin{smallmatrix}4_2\\q\end{smallmatrix}\right)$	
		$m=2n$:	$\left(\begin{smallmatrix}4\\s\end{smallmatrix}\right)$	$m=4n$:	$\left(\begin{smallmatrix}4\\q\end{smallmatrix}\right)$			
$HHLm$	**a** − **b**‡	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$	$2H+L-4n$:	$\left(\begin{smallmatrix}d\\1\end{smallmatrix}\right)$	
Trigonal/hexagonal								
$00Lm$	**c**	$L=2n$:	$\left(\begin{smallmatrix}6_3\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}6\\s\end{smallmatrix}\right)$	$L=3n$:	$\left(\begin{smallmatrix}3_1\\1\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}6_2\\1\end{smallmatrix}\right)$	
		$L=6n$:	$\left(\begin{smallmatrix}6_1\\1\end{smallmatrix}\right)$	$2L+m=6n$:	$\left(\begin{smallmatrix}6_2\\h\end{smallmatrix}\right)$	$m=3n$:	$\left(\begin{smallmatrix}3\\t\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}6\\t\end{smallmatrix}\right)$	
		$m=6n$:	$\left(\begin{smallmatrix}6\\h\end{smallmatrix}\right)$	$3L+m=6n$:	$\left(\begin{smallmatrix}6_3\\h\end{smallmatrix}\right)$			
$0KLm$	**a**§	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$	$L+m=2n$:	$\left(\begin{smallmatrix}c\\s\end{smallmatrix}\right)$	
$HHLm$	**a** − **b**	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$	$L+m=2n$:	$\left(\begin{smallmatrix}c\\s\end{smallmatrix}\right)$	

† Bravais class 11

$0KLm$	**a**	$K+m=4n$:	$\left(\begin{smallmatrix}b\\q\end{smallmatrix}\right)$	$K+2L+m=4n$:	$\left(\begin{smallmatrix}n\\q\end{smallmatrix}\right)$
$HK00$	**c**	$H+K=4n$:	$\left(\begin{smallmatrix}n\\\bar{1}\end{smallmatrix}\right)$		

‡ Bravais class 20

$0KLm$	**a** − **b**	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$		
$HHLm$	**a**	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$L+m=2n$	$\left(\begin{smallmatrix}c\\s\end{smallmatrix}\right)$	$2H+m=4n$:	$\left(\begin{smallmatrix}b\\q\end{smallmatrix}\right)$
		$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$			$2H+2L+m=4n$:	$\left(\begin{smallmatrix}n\\q\end{smallmatrix}\right)$

§ Bravais class 23

$0KLm$	**2a** − **b**	$L=2n$:	$\left(\begin{smallmatrix}c\\1\end{smallmatrix}\right)$	$m=2n$:	$\left(\begin{smallmatrix}m\\s\end{smallmatrix}\right)$

Hence there are systematic extinctions for $H + K + m$ odd. The conditions for the 24 Bravais classes are given in Table 1.

Next to these general conditions, there are special ones due to the translational parts of symmetry operations. If $f(\mathbf{H})$ is the Fourier transform of the (electron) density function of an incommensurate structure which is invariant under the transformation (3.1–3.2), one has the following relation for $\mathbf{H}$ given by (5.1):

$$f(\mathbf{H}) = f(R\mathbf{H}) \exp\{2\pi i[R\mathbf{H}.\mathbf{s} + \varepsilon m(\delta - \mathbf{q}.\mathbf{s})]\}. \tag{5.9}$$

This simply expresses the invariance in reciprocal space. So, if $R\mathbf{H} = \mathbf{H}$ and $\varepsilon = +1$, a condition for nonvanishing Fourier components is

$$\mathbf{H}.\mathbf{s} + m(\delta - \mathbf{q}.\mathbf{s}) = n, \quad n \text{ integer}. \tag{5.10}$$

The translation $\mathbf{s}$ may be expressed in components with reference to $\mathbf{a}_s$, $\mathbf{b}_s$, $\mathbf{c}_s$:

$$\mathbf{s} = x\mathbf{a}_s + y\mathbf{b}_s + z\mathbf{c}_s. \tag{5.11}$$

Then (5.10) can be expressed in terms of τ (3.8):

$$Hx + Ky + Lz + m\tau = n, \tag{5.12}$$

which is no longer explicitly dependent on the Bravais type. The symbol for the superspace group contains information about those x, y, z and τ values which cannot be transformed to zero by a change of origin.

As an example we take the superspace group $W^{P4bm}_{qq\,1}$ which contains an element $\binom{b}{q}$ with

$$R = m_x, \quad \varepsilon = 1, \quad \mathbf{s} = \tfrac{1}{2}\mathbf{b} = \tfrac{1}{4}(\mathbf{a}_s + \mathbf{b}_s), \quad \tau = \tfrac{1}{4}. \tag{5.13}$$

The vector $\mathbf{H}$ (5.1) is left invariant if $H = K$. Then the spots are only nonvanishing if (5.12) is satisfied:

$$\frac{H + K + m}{4} = n. \tag{5.14}$$

So the condition for the diffraction spots corresponding to the existence of the symmetry element (5.13) is $H + K + m = 4n$. This and the other conditions due to nonprimitive translations are given in Table 3.

6. Determination

To determine the complete list of superspace groups, we have used two independent methods. Both start with the determination of the Bravais types: for each three-dimensional crystallographic point group it is checked if there is an incommensurate vector $\mathbf{q}$ satisfying (3.4) for all group elements combined with a factor ε. Since basic lattice and vector $\mathbf{q}$ determine the lattice in R_4, the Bravais types are then found using the definitions from § 4. In the first method, for each holohedral point group the nonequivalent subgroups are determined, yielding the arithmetic crystal classes. The superspace groups are extensions in the group-theoretical sense of the point group with a four-dimensional translation group. For one representative point group from each arithmetic crystal class all nonequivalent superspace groups are then found with an algorithm developed for n-dimensional space groups. The same algorithm has been used by Fast & Janssen (1968). The difference between this work and that of Fast & Janssen is that here only a part of all point groups describe incommensurate structures and one has to implement another (stronger) equivalence criterion.

The second method uses the fact that each superspace group is isomorphic – modulo integer increments of t – with its basic space group. Hence, it can be formed, like the latter, by a synthesis running parallel to the well-known construction of point groups through subsequent enlargement of the set of generators. For instance,

		added		added	
point groups	4	(m)	$4/m$	(m)	$4/mmm$
space groups	$P4$	(n)	$P4/n$	(m)	$P4/nbm$
International Tables for X-ray Crystallography number	75		85		125
superspace groups	$W^{P4}_{?}$	$\binom{n}{\bar{1}}$	$W^{P4/n}_{?\,\bar{1}}$	$\binom{m}{?}$	$W^{P4/nbm}_{?\,\bar{1}??}$

Such pedigrees fulfil the condition that the added element transforms into itself the group to which it is added. A superspace group is determined completely by the basic space group, one element with $\varepsilon = -1$ and all the other ones with $\varepsilon = +1$ (that is, those which do not invert $\mathbf{q}_i$). It is sufficient to find the values of τ for the latter elements only, as indicated above by a question mark, because the τ of the chosen element with $\varepsilon = -1$ can always be taken as zero. The question marks can be filled in by checking the above condition for the t part of the relevant operations $g = (R, \varepsilon, \mathbf{s}, \tau)$, using the following relations:

$$\text{if } g_1 g_2(\mathbf{r}, t) = g_3(\mathbf{r}, t)\text{: } \varepsilon_3 = \varepsilon_1 \varepsilon_2, \ \tau_3 = \tau_1 + \varepsilon_1 \tau_2 \tag{6.1}$$

$$\text{if } g_2^{-1} g_1 g_2(\mathbf{r}, t) = g_1'(\mathbf{r}, t)\text{: } \varepsilon_1' = \varepsilon_1,$$

$$\tau_1' = \varepsilon_2 \tau_1 + \varepsilon_2(\varepsilon_1 - 1)\tau_2. \tag{6.2}$$

In the transformation (6.2), only the case $\varepsilon_1 = +1$ is needed; then

$$\tau_1' = \varepsilon_2 \tau_1. \tag{6.3}$$

In the above example, the group $P4$ has two inequivalent axes. A rotation (R_1) of $\pi/2$ around one axis, multiplied by a translation $(\mathbf{s}_2)$ along $\mathbf{a}$ yields a $\pi/2$ rotation (R_3) about the other axis. Since in the Bravais class no. 20 ($W^{P4/mmm}_{1\,\bar{1}\,1\,1}$), the vector $\mathbf{q}$ is of the form

$(\frac{1}{2}\frac{1}{2}\gamma)_*$, the translation **a** has a t part $\tau_2 = \frac{1}{2}$. Accordingly, (6.1) with $g_1 = (R_1, \varepsilon_1 = 1, \mathbf{s} = 0, \tau_1 = ?)$ and $g_2 = (1, 1, \mathbf{a}, \tau_2 = \frac{1}{2})$ gives

$$\tau_3 = \tau_1 + \tfrac{1}{2}. \qquad (6.4)$$

Since g_1 is of order 4, the possible τ_1 values are 0, $\frac{1}{4}$ or $\frac{1}{2}$ and we have $(\tau_1, \tau_3) = (0, \frac{1}{2})$, $(\frac{1}{2}, 0)$ or $(\frac{1}{4}, -\frac{1}{4})$. The first two are equivalent (superspace group 75.20.1), the last is 75.20.2.

Adding the n mirror with $\varepsilon = -1$, we note that it transforms g_1 and g_3 into each other. By (6.3), this requires $\tau_3 = -\tau_1$, which rules out the $(0, \frac{1}{2})$ case, leaving only $(\frac{1}{4}, -\frac{1}{4})$: 85.20.3. Finally, a mirror plane parallel to the fourfold axes is added to obtain no. 125, for instance the diagonal m plane. From the spatial configuration (m lies between the axes) it follows that m transforms g_1 into g_3^{-1}. According to (6.3) this gives $\tau_3 = -\tau_1' = -\tau_1$, which agrees with the former result independently of the τ assigned to m. Hence, τ can be either 0 (125.20.5) or $\frac{1}{2}$ (125.20.6). Since the mirror b in $P4/nbm$ is the product of m and g_1, (6.1) yields $\tau = \pm\frac{1}{4}$ for b, so the complete pedigree becomes:

space group	$P4$	$P4/n$	$P4/nbm$
possible superspace groups	W_1^{P4}		
	W_q^{P4}	$\rightarrow W_{q\,\bar{1}}^{P4/n}$	$\rightarrow W_{q\,\bar{1}q1}^{P4/nbm}$
			$\rightarrow W_{q\,\bar{1}qs}^{P4/nbm}$

Of course, different lines of ascendence are possible, such as $P4 - P4bm - P4/nbm$, to arrive at no. 125, which is in the most complicated arithmetic class of all; the derivation of the majority of superspace groups is simpler than in the above example.

References

AALST, W. VAN, DEN HOLLANDER, J., PETERSE, W. J. A. M. & DE WOLFF, P. M. (1976). *Acta Cryst.* B**32**, 47–58.

BAK, P. & JANSSEN, T. (1978). *Phys. Rev.* B**17**, 436–439.

BROWN, H., BÜLOW, R., NEUBÜSER, J., WONDRATSCHEK, H. & ZASSENHAUS, H. (1978). *Crystallographic Groups of Four-Dimensional Space*. New York: Wiley.

FAST, G. & JANSSEN, T. (1968). Report 6-68, Univ. of Nijmegen, The Netherlands.

International Tables for X-ray Crystallography (1969). Vol. I, edited by N. F. M. HENRY & K. LONSDALE. Birmingham: Kynoch Press.

JANNER, A. & JANSSEN, T. (1977). *Phys. Rev. B*, **15**, 643–658.

JANNER, A. & JANSSEN, T. (1979). *Physica (Utrecht)*, **99**A. 47–76.

JANNER, A. & JANSSEN, T. (1980*a*). *Acta Cryst.* A**36**, 399–408.

JANNER, A. & JANSSEN, T. (1980*b*). *Acta Cryst.* A**36**, 408–415.

JANNER, A., JANSSEN, T. & DE WOLFF, P. M. (1979). *Proceedings of the Conference on Modulated Structures*, edited by J. M. COWLEY, J. B. COHEN, M. B. SALAMON & B. J. WUENSCH. *AIP Conf. Proc.* **53**, 81–83.

JANSSEN, T. (1979). *J. Phys. C*, **12**, 5381–5392.

JANSSEN, T., JANNER, A. & DE WOLFF, P. M. (1980). *Proceedings of the Conference on Group Theoretical Methods in Physics, Zvenigorod, USSR*, November 1979.

JOHNSON, C. K. & WATSON, C. R. (1976). *J. Chem. Phys.* **64**, 2271–2286.

VALENTINE, D. Y., CAVIN, O. B. & YAKEL, H. L. (1977). *Acta Cryst.* B**33**, 1389–1396.

WOLFF, P. M. DE (1974). *Acta Cryst.* A**30**, 777–785.

WOLFF, P. M. DE (1977). *Acta Cryst.* A**33**, 493–497.

YAMAMOTO, A., NAKAZAWA, H. & TOKONAMI, M. (1979). *Proceedings of the Conference on Modulated Structures*, edited by J. M. COWLEY, J. B. COHEN, M. B. SALAMON & B. J. WUENSCH. *AIP Conf. Proc.* **53**, 84–86.

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Optimum Choice of Wavelengths in the Anomalous Scattering Technique with Synchrotron Radiation

BY RAMESH NARAYAN

Raman Research Institute, Bangalore 560080, *India*

AND S. RAMASESHAN

Indian Institute of Science, Bangalore 560012, *India*

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Abstract

A formula has been derived for the mean-square error in the phases of crystal reflections determined through the multiwavelength anomalous scattering method. The error is written in terms of a simple function of the positions in the complex plane of the 'centres' corresponding to the different wavelengths. For the case of three centres, the mean-square error is inversely proportional to the area of the triangle formed by them.

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