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## Bravais Classes for Incommensurate Crystal Phases

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### Abstract

A full classification is given of the Bravais classes of lattices of symmetry groups of incommensurate crystal phases with an internal (additional) dimensionality  $d$  lower than four. These Bravais classes form the basis for the derivation of superspace groups needed for the symmetry classification of incommensurate crystal phases. By means of examples it is indicated how the information contained in the various tables can be extracted and used, for example, for the derivation of superspace groups.

### I. Introduction

An incommensurate crystal is characterized by the occurrence of at least four periodicities, three of which describe a usual crystal structure, whereas the additional ones are incommensurate with the former ones. Because of the incommensurability there is no three-dimensional lattice translation symmetry. It has been shown, however, that nevertheless the appropriate symmetry group for such a case is a crystallographic space group, not in three but in  $3 + d$  dimensions (de

Wolff, 1974, 1977; Janner & Janssen, 1977), a so-called superspace group. The additional dimension can be interpreted as an internal degree of freedom.

For the simplest case of one additional dimension, the inequivalent  $(3 + 1)$ -dimensional superspace groups have been tabulated together with the corresponding classes of Bravais lattices (de Wolff, Janssen & Janner, 1981). However, there are also examples of crystal phases with an internal dimensionality higher than one. Since it has been shown that in general  $(3 + d)$ -dimensional superspace groups are useful for the classification and for the structure analysis of three-dimensional crystal phases (e.g. Yamamoto, 1982), it is of relevance to investigate these higher-dimensional superspace groups, also. The number of superspace groups, however, increases rapidly with increasing dimension and easily exceeds the number of known incommensurate crystal phases. Therefore, it does not seem to make sense to work out a complete list.

The number of Bravais classes on the other hand is much more restricted. Moreover, they form the basis for the determination of superspace groups and provide a useful framework for their classification. In the present paper we discuss the general theory and give a derivation of a complete list of classes with internal dimension up to three.

This list covers all cases of incommensurate crystal phases known so far. In a subsequent paper (Janner, Janssen & de Wolff, 1983*b*) we show how, on the basis of the present list and knowing the geometrical arrangement of the diffraction pattern of a given crystal, one can easily identify the Bravais class of that crystal.

Crystallographers not interested to know how one gets (for a given internal dimension) all the Bravais classes may skip most of the present article and learn in the paper mentioned above how to use the tables for practical cases.

Three is not the maximal internal dimension which can occur in incommensurate crystals. In phase transitions leading to a modulated crystal one often sees the condensation of elementary excitations (phonons). One can distinguish cases where these are independent and others where they are related by symmetry. In the latter case the wave vectors form a so-called 'star'. Bravais classes associated with a single star of additional (satellite) wave vectors are called elementary Bravais classes (EBC's). The more general case is then obtained by superposition of stars. The concept of EBC plays a role in the present paper, but EBC's are discussed in more detail and derived in another paper (Janner, Janssen & de Wolff, 1983*a*). The reason is that (most of) the EBC's allow another type of derivation based on Wyckoff positions of centrosymmetric symmorphic space groups. They can thus be read off from *International Tables for X-ray Crystallography* (1969) (referred to as IT).

Coming back to the present paper we recall that the classification of superspace groups is based on the arithmetic crystal classes. By means of a number of examples we indicate how one can derive such crystal classes from the Bravais classes, and moreover illustrate the determination of superspace groups. In the situation where enough structural information on a given crystal phase is available, by looking at those examples and on the basis of the tables presented here, it should be possible to identify the superspace group describing the symmetry of that crystal.

## II. Lattice symmetry of incommensurate crystal phases

The reflections in X-ray or neutron scattering from an incommensurate crystal phase can be labeled by a set of integers (indices), but need for their labeling more than three indices. An arbitrary wave vector describing such a reflection can be written as, for example,

$$\mathbf{k} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}_j^*, \quad (1)$$

or in a more compact form, and more generally, as

$$\mathbf{k} = \sum_{i=1}^3 h_i \mathbf{a}_i^* + \sum_{j=1}^d m_j \mathbf{q}_j^*. \quad (2)$$

Here the vectors  $\mathbf{q}_1^*, \dots, \mathbf{q}_d^*$ , which are called modulation wave vectors, are chosen in such a way that the vectors  $\mathbf{a}_1^*, \dots, \mathbf{q}_d^*$  are rationally independent and that the reflections with  $m_j = 0$  (all  $j$ ) are the so-called main reflections; the other ones being the corresponding satellites. The main reflections belong to a three-dimensional reciprocal lattice  $\mathcal{A}^*$  spanned by  $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ . The set of all vectors of the form (2) with arbitrary integers  $h_i, m_j$  is here denoted by  $M^*$ .

Because the vectors  $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$  form a basis for the three-dimensional real space, called external or positional and denoted by  $V_E$ , the modulation wave vectors  $\mathbf{q}_j^*$  can be expressed as a linear combination of them:

$$\mathbf{q}_j^* = \sum_{i=1}^3 \sigma_{ji} \mathbf{a}_i^*. \quad (3)$$

The condition of rational independence means that in each row of the  $d \times 3$ -dimensional matrix  $\sigma$  there is at least one irrational entry, or even stronger: in every linear combination with integral coefficients of the rows of  $\sigma$  there is such an irrational entry.

Let us denote the (holohedral) point group of  $\mathcal{A}^*$  by  $K_{\mathcal{A}}$ . If  $\mathcal{A}$  is the direct lattice corresponding to  $\mathcal{A}^*$ , i.e. the lattice generated by  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  with

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \quad (4)$$

then  $K_{\mathcal{A}}$  is also the point group of  $\mathcal{A}$ .

Now we consider the group  $K$  of all elements of  $K_{\mathcal{A}}$  which leave  $M^*$  invariant. Because  $K$  is a subgroup of  $K_{\mathcal{A}}$ , the lattice  $\mathcal{A}^*$  is left invariant by any element  $R$  of  $K$ : the transformed vector  $R\mathbf{a}_i^*$  is a linear combination of the basis vectors  $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ . Thus

$$R\mathbf{a}_i^* = \sum_{j=1}^3 c_{ij} \mathbf{a}_j^*, \quad i = 1, 2, 3. \quad (5)$$

The integral coefficients  $c_{ij}$  form a  $3 \times 3$ -dimensional matrix that we shall denote by  $\Gamma_E(R^{-1})$ . We use here  $\Gamma_E(R^{-1})$  rather than  $\Gamma_E(R)$  because the transformation acts in reciprocal space. In this way agreement is obtained with Janner & Janssen (1979). The vectors  $\mathbf{q}_j^*$  transform under  $R$  of  $K$  into vectors of the form (2), i.e.

$$R\mathbf{q}_j^* = \sum_{i=1}^3 \Gamma_M(R^{-1})_{ji} \mathbf{a}_i^* + \sum_{k=1}^d \Gamma_I(R^{-1})_{jk} \mathbf{q}_k^*, \quad (6)$$

$$j = 1, \dots, d.$$

The integral coefficients  $\Gamma_M(R^{-1})_{ji}$  and  $\Gamma_I(R^{-1})_{jk}$  form matrices of dimension  $d \times 3$  and  $d \times d$ , respectively. The latter, because of the condition of rational independence, are invertible and they form a finite group. According to a theorem of algebra, this group is equivalent to a group of orthogonal matrices. In other words, in the  $d$ -dimensional real space  $R^d$  there are orthogonal transformations  $R_I$  and a basis  $\mathbf{b}_1^*, \dots, \mathbf{b}_d^*$  (in general not orthogonal) such that

$$R_I \mathbf{b}_k^* = \sum_{l=1}^d \Gamma_I(R^{-1})_{kl} \mathbf{b}_l^*. \quad (7)$$

We call this Euclidean space the internal space and denote it by  $V_I$ . The lattice spanned by  $\mathbf{b}_1^*, \dots, \mathbf{b}_d^*$  is left invariant by  $R_I$  (one for each  $R$  of  $K$ ) and the same is true for the lattice spanned by the dual basis  $\mathbf{b}_1, \dots, \mathbf{b}_d$ .

One can now consider the direct sum space  $V_S$  of  $V_E$  and  $V_I$ . In this space (which we take to be also Euclidean) there exists a lattice  $\Sigma^*$  spanned by  $3 + d$  vectors:

$$\begin{aligned} \mathbf{a}_i^* &= (\mathbf{a}_i^*, 0), \quad i = 1, 2, 3 \\ \mathbf{a}_{3+j}^* &= (\mathbf{q}_j^*, \mathbf{b}_j^*), \quad j = 1, \dots, d. \end{aligned} \quad (8)$$

Here vectors in ordinary three-dimensional space and in internal space are denoted by a bold face symbol. As a consequence of (5–7) the lattice  $\Sigma^*$  is left invariant by a group of orthogonal transformations such that  $\mathbf{a}_i^*$  is transformed into

$$\mathbf{a}_i'^* = \sum_{j=1}^{3+d} \Gamma(R^{-1})_{ij} \mathbf{a}_j^* \quad (R \text{ in } K), \quad (9)$$

where the matrix  $\Gamma(R)$  is

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix}. \quad (10)$$

The dual lattice  $\Sigma$  in the  $(3 + d)$ -dimensional space is spanned by

$$\begin{aligned} \mathbf{a}_i &= (\mathbf{a}_i, -\Delta \mathbf{a}_i), \quad i = 1, 2, 3, \\ \mathbf{a}_{3+j} &= (0, \mathbf{b}_j), \quad j = 1, \dots, d, \end{aligned} \quad (11)$$

where the components of  $\mathbf{a}_i$  in the internal space are given by

$$\Delta \mathbf{a}_i = \sum_{j=1}^d \sigma_{ji} \mathbf{b}_j. \quad (12)$$

The matrix  $\sigma$  in (12) is exactly the same as that appearing in (3). As we have discussed in Janner & Janssen (1977), the internal space  $V_I$  corresponds to  $d$  degrees of freedom, which can be interpreted as the phases of the modulation in the case of a displacively modulated crystal. As we have shown in Janner & Janssen (1980), the symmetry of incommensurate crystal phases can be described by superspace groups (Janner & Janssen, 1979), which are  $(3 + d)$ -dimensional space groups with a lattice spanned by vectors as in (11) and point groups  $K$  constructed as indicated above.

This is the reason why crystallographic concepts can be applied to incommensurate crystal phases as well, and why it makes sense to study the Bravais classes of  $(3 + d)$ -dimensional lattices.

### III. Classes of Bravais lattices

The lattice  $\Sigma$  is completely determined by the basis vectors  $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*, \mathbf{q}_1^*, \dots, \mathbf{q}_d^*$  of  $M^*$  (up to the freedom one has in the choice of the basis  $\mathbf{b}_1, \dots, \mathbf{b}_d$ ).

Equivalently it is determined by  $\mathbf{a}_i^*$  ( $i = 1, 2, 3$ ) and the matrix  $\sigma$ . Here we want to discuss the question when two lattices  $\Sigma$  and  $\Sigma'$  can be called equivalent.

For given basis  $\mathbf{a}_i^*, \mathbf{q}_j^*$  ( $i = 1, 2, 3; j = 1, \dots, d$ ) an element  $R$  of  $K$  gives rise to an orthogonal transformation which has the form  $\Gamma(R)$  of (10) with respect to the basis (8). Moreover, if  $R_1$  and  $R_2$  are elements of  $K$  then

$$\Gamma(R_1 R_2) = \Gamma(R_1) \Gamma(R_2), \quad (13)$$

*i.e.*  $\Gamma$  is a group homomorphism. If we restrict ourselves to orthogonal transformations  $(R_E, R_I)$  in  $V_S$  leaving both subspaces  $V_E$  and  $V_I$  invariant but otherwise arbitrary, then every transformation leaving  $\Sigma^*$  (or  $\Sigma$ ) invariant is of the form (10). This can be seen as follows. Suppose  $(1, R_I)$  leaves  $\Sigma^*$  invariant. Take an element  $\mathbf{k} = (\mathbf{k}_E, \mathbf{k}_I)$  from  $\Sigma^*$ , where  $\mathbf{k}_E$  is of the form (2) and  $\mathbf{k}_I = \sum_j m_j \mathbf{b}_j^*$ . Then  $(\mathbf{k}_E, R_I \mathbf{k}_I)$  is an element of  $\Sigma^*$  and  $\mathbf{k}_E$  belongs to  $M^*$ . Because of the condition of rational independence, there is exactly one element from  $\Sigma^*$  for each element of  $M^*$ , and thus one single  $\mathbf{k}_I$  for each  $\mathbf{k}_E$ . This means that  $R_I \mathbf{k}_I = \mathbf{k}_I$ . Because  $\mathbf{k}_E$ , and accordingly  $\mathbf{k}_I$  are arbitrary, this implies that  $R_I = 1$ . In other words,  $\Gamma$  is even an isomorphism: there is exactly one  $\Gamma(R)$  for each  $R$  in  $K$  and if  $(R_E, R_I)$  leaves  $\Sigma$  invariant then  $R_E$  belongs to  $K$ . One can call  $K$  the (holohedral) point group of  $\Sigma^*$  (and of  $\Sigma$ ). The restriction to pairs  $(R_E, R_I)$  means that we only consider transformations which map vectors of  $\Sigma^*$  corresponding to main reflections to similar ones, and that the point group  $\Gamma(K)$  consisting of matrices  $\Gamma(R)$  is  $3 + d$  reducible, *i.e.* there is a basis in  $V_S$  such that these matrices are of the form (10) with  $\Gamma_M = 0$ . We do not consider as symmetry transformations the so-called irreducible ones, which mix internal and external coordinates. At present no crystals are known where such irreducible symmetries in dimensions higher than three can be applied.

Just as in ordinary three-dimensional crystallography, we call two lattices  $\Sigma$  and  $\Sigma'$  of the same Bravais class if there are (primitive) bases such that the corresponding holohedral point groups are represented by the same group of matrices. The only difference with ordinary crystallography is that the class of allowed basis transformations is in the present case restricted to those leaving the reduced matrix form (10) invariant.

Suppose the basis  $\mathbf{a}_i^*, \mathbf{q}_j^*$  of  $M^*$  gives rise to the group of matrices  $\Gamma(R)$  as above. A new basis of  $M^*$  keeping the integral indices labeling can then be expressed in terms of integral linear combination of the original basis elements:

$$\begin{aligned} \mathbf{c}_i^* &= \sum_{j=1}^3 S_{ij} \mathbf{a}_j^*, \quad i = 1, 2, 3, \\ \mathbf{r}_j^* &= \sum_{k=1}^d T_{jk} \mathbf{q}_k^* + \sum_{i=1}^3 U_{ji} \mathbf{a}_i^*, \quad j = 1, \dots, d, \end{aligned} \quad (14)$$

where  $S_{ij}$  and  $T_{jk}$  are the entries of unimodular matrices  $S$  and  $T$ , respectively. So the first three basis vectors again describe main reflections. Starting from the basis (14) one obtains a lattice  $\Sigma'^*$  and matrices

$$\Gamma'(R) = \begin{pmatrix} \Gamma'_E(R) & 0 \\ \Gamma'_M(R) & \Gamma'_I(R) \end{pmatrix} \quad (R \text{ in } K) \quad (15)$$

with

$$\begin{aligned} \Gamma'_E(R) &= S\Gamma_E(R)S^{-1}, & \Gamma'_I(R) &= T\Gamma_I(R)T^{-1} & (16) \\ \Gamma'_M(R) &= T\Gamma_M(R)S^{-1} + V\Gamma'_E(R) - \Gamma'_I(R)V \\ & & (V &= US^{-1}). & (17) \end{aligned}$$

Hence lattices  $\Sigma$  and  $\Sigma'$  may only belong to the same Bravais class if the groups  $\Gamma_E(K)$  and  $\Gamma'_E(K)$  and  $\Gamma_I(K)$  and  $\Gamma'_I(K)$  are arithmetically equivalent. Moreover, there has to exist an integral  $d \times 3$ -dimensional matrix  $V$  such that (17) is also satisfied. The latter equation, actually, can be translated as follows into a condition on the matrices  $\sigma$  and the corresponding  $\sigma'$ . Equation (17) implies for the matrices  $\sigma$  and  $\sigma'$  the relation:

$$\sigma' = T\sigma S^{-1} + V. \quad (18)$$

The relation between  $\Gamma_M, \Gamma_E, \Gamma_I$  and  $\sigma$  is

$$\sigma\Gamma_E(R) - \Gamma_I(R)\sigma = \Gamma_M(R), \quad (19)$$

as follows from (2) and (3); and correspondingly for the primed elements also. This relation puts restrictions on the possible matrices  $\sigma$  for given  $\Gamma_E(K)$  and  $\Gamma_I(K)$ , because  $\Gamma_M(R)$  is an integral matrix. It can be shown that the matrix  $\sigma$  can be written as a sum  $\sigma = \sigma^i + \sigma^r$ , where  $\sigma^i$  satisfies an equation similar to (19), but with zero at the right-hand side:

$$\sigma^i \Gamma_E(R) - \Gamma_I(R)\sigma^i = 0 \quad (\text{all } R \text{ in } K) \quad (20)$$

and where  $\sigma^r$  is a matrix with rational entries. Hence the restricting equation (19) becomes

$$\sigma^r \Gamma_E(R) - \Gamma_I(R)\sigma^r = \Gamma_M(R). \quad (21)$$

The freedom and the restrictions one has in the lattices of a Bravais class for a given  $M^*$  also apply to lattices constructed from different reflection sets  $M^*$  and  $M^{**}$ . Accordingly we are now in a position to formulate criteria for deciding whether two lattices  $\Sigma$  and  $\Sigma'$  belong to the same Bravais class.

Consider any two lattices  $\Sigma$  and  $\Sigma'$  with holohedral point groups  $K$  and  $K'$ , respectively, and their integral (faithful) representations  $\Gamma(K)$  and  $\Gamma'(K')$ . Then the two lattices belong to the same Bravais class if and only if

$$\Gamma'(K') = A\Gamma(K)A^{-1}, \quad (22)$$

where the  $(3+d) \times (3+d)$ -dimensional matrix  $A$  with integral entries and determinant  $\pm 1$  has the form

$$A = \begin{pmatrix} S & 0 \\ U & T \end{pmatrix}. \quad (23)$$

This implies in particular that  $K$  and  $K'$  are isomorphic point groups, and can be here identified.

If the lattices are given by bases  $\mathbf{a}_i^*$ ,  $\mathbf{q}_j^*$  of  $M^*$  and  $\mathbf{a}_i^{**}$ ,  $\mathbf{q}_j^{**}$  of  $M^{**}$ , the ensuing lattices  $\Sigma$  and  $\Sigma'$  are of the same Bravais class if there is a basis transformation as in (14) such that the set of matrices  $\Gamma_E(R)$ ,  $\Gamma_I(R)$  and  $\Gamma_M(R)$  are correspondingly the same for both lattices.

If the lattices are given by  $\mathbf{a}_i^*$  and  $\sigma$ , and by  $\mathbf{a}_i^{**}$  and  $\sigma'$ , the lattices belong to the same Bravais class if  $\Gamma_E(K)$  is arithmetically equivalent *via* a matrix  $S$  to  $\Gamma_E'(K)$ , i.e. one can perform a basis transformation with matrix  $S$  on the basis  $\{\mathbf{a}_i^*\}$  such that the (holohedral) point groups become of the same form, and furthermore there is a matrix  $T$  with integral entries such that

$$\sigma' \equiv T\sigma S^{-1} \quad (\text{modulo integers}). \quad (24)$$

#### IV. Notation

One way to characterize a Bravais class is to give the arithmetic crystal class of  $\Gamma(K)$ . This can be done by indicating the arithmetic crystal classes of  $\Gamma_E(K)$  and  $\Gamma_I(K)$ , their mutual correspondence as pairs appearing in  $\Gamma(K)$ , and  $\sigma^r$ . Then the Bravais class is given by a two-line symbol. The top line indicates the arithmetic crystal class of  $\Gamma_E(K)$  in the form of the symbol one finds in IT for its associated symmorphic space group. The bottom line gives the arithmetic crystal class of  $\Gamma_I(K)$ , also by its IT symbol. The latter implies a restriction to  $d = 1, 2$  and  $3$ . The arrangement of top and bottom lines is such that paired elements are one above the other. This may require a permutation in the elements appearing in the IT symbol. Moreover, if  $R_I \neq 1$  then necessarily  $R \neq 1$ , but if  $R_I = 1$  it is also possible to have  $R \neq 1$ . If  $R$  appears as an element of the symbol and  $R_I = 1$ , then a 1 is added correspondingly in the bottom line. Finally, the matrix  $\sigma^r$  is indicated in the form of a prefix. For  $d = 1$  a systematic for this prefix has been developed (*cf.* Janner, Janssen & de Wolff, 1979), but for larger values of  $d$  we have chosen a simpler system, to avoid a too complicated casuistry. Accordingly,  $P$  just means:  $\sigma^r = 0$ , whereas the other possible matrices are labeled  $C_1, C_2, \dots$ , etc. As suggested by the notation the lattices with a  $C_i$  prefix are centerings of the corresponding  $P$  ones.

As an example consider some of the cases in which the main reflections form a monoclinic primitive lattice:

(i) Two of the basic satellites lie in the mirror plane  $z = 0$  and a third one lies along the unique axis; then the matrix  $\sigma$  is identical with  $\sigma^i$  and

$$\sigma = \begin{pmatrix} \alpha & \beta & 0 \\ \sigma = \lambda & \mu & 0. \\ 0 & 0 & \theta \end{pmatrix}. \quad (25)$$

Since all elements of  $2/m$  leave  $M^*$  invariant:  $K = 2/m$ . Also from (6) it follows for this case that  $K_I = 2/m$  and that the four elements of the  $(3 + 3)$ -dimensional point group are:  $(1,1)$ ,  $(2,2)$ ,  $(m,m)$  and  $(-1,-1)$ . Finally,  $\sigma^r = \sigma - \sigma^i = 0$ . Hence the two-line symbol is:

$$P_{P2/m}^{P2/m}$$

(ii) Two of the basic satellites lie along the unique axis and a third one in the mirror plane. Again,  $K = K_E = 2/m$  and  $K_I = 2/m$ . However, now the four elements of the  $(3 + 3)$ -dimensional point group are:  $(1,1)$ ,  $(2,m)$ ,  $(m,2)$  and  $(-1,-1)$ . The corresponding symbol is

$$P_{Pm/2}^{P2/m}$$

(iii) A non-vanishing  $\sigma^r$  is obtained if one basic satellite lies in the mirror plane at  $z = \frac{1}{2}$ , one in the mirror plane at  $z = 0$  and a third along the unique axis. Then

$$\begin{array}{cccccc} \alpha & \beta & 0 & & 0 & 0 & \frac{1}{2} \\ \sigma^i = \lambda & \mu & 0 & & \sigma^r = 0 & 0 & 0 \\ 0 & 0 & \theta & & 0 & 0 & 0 \end{array}$$

In this case the elements of  $K$  are, as in the first one:  $(1,1)$ ,  $(2,2)$ ,  $(m,m)$  and  $(-1,-1)$ , but since  $\sigma^r \neq 0$ , the symbol for this third case is

$$C_{1P2/m}^{P2/m}$$

Another notation for the classes of Bravais lattices, which is more compact and can be used for  $d > 3$  also, is based on the fact that the lattice  $\Sigma$  is given once one knows the vectors  $\mathbf{a}_i^*$  and  $\mathbf{q}_j^*$ . The arithmetic crystal class of  $\Gamma_E(K)$  is again indicated by its IT symbol. The additional required information can, for example, be given by indicating the components of the vectors  $\mathbf{q}_j^*$  with respect to the basis adopted in IT for  $\Gamma_E(K)$ : in other words one gives in this way the matrix  $\sigma$ . However, this information is, in general, redundant. Because of (6) the vectors  $\mathbf{q}_j^*$  are transformed among each other (up to vectors of  $A^*$ ) by the elements of  $K$ . This means that there are vectors  $\mathbf{Q}_1^*, \dots, \mathbf{Q}_p^*$  such that the set of vectors  $R\mathbf{Q}_i^*$  for all  $R$  of  $K$  and  $i = 1, \dots, p$ , generate together with  $\mathbf{a}_1^*, \mathbf{a}_2^*$  and  $\mathbf{a}_3^*$  the set  $M^*$  of all reflections. In the worst case  $p = d$ , but usually  $p$  may take a much smaller value. In particular it may happen that  $p = 1$ : there are just one single vector  $\mathbf{Q}^*$  and  $d$  elements  $R_j$  of  $K$  such that:

$$\mathbf{q}_j^* \equiv R_j \mathbf{Q}^* \quad (\text{up to vectors of } A^*), \quad j = 1, \dots, d. \quad (26)$$

A Bravais class for which this choice is possible is called an elementary Bravais class. In the language of solid-state theory one says that all basic satellites (*i.e.* all modulation wave vectors)  $\mathbf{q}_j^*$  belong to one star of  $K$ .

In a non-elementary  $(3 + d)$ -dimensional Bravais class the vectors  $\mathbf{Q}_i^*$  can be chosen among the vectors of different stars. In that case next to the arithmetic

crystal class of  $\Gamma_E(K)$ , it is sufficient to give the components of the  $\mathbf{Q}_k^*$  ( $k = 1, \dots, p$ ) with respect to the basis adopted in IT. The symbol is then of the form  $\Gamma_E(K)$  ( $\mathbf{Q}_1^*, \dots, \mathbf{Q}_p^*$ ), and can be more convenient than the two-line symbol.

As an example we consider the case that  $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$  span a primitive tetragonal lattice. Suppose  $d = 2$  and  $\mathbf{q}_1^* = \alpha\mathbf{a}_1^* + \beta\mathbf{a}_2^* = (\alpha, \beta, 0)$ ;  $\mathbf{q}_2^* = -\beta\mathbf{a}_1^* + \alpha\mathbf{a}_2^* = (-\beta, \alpha, 0)$ . The subgroup of the holohedral point group  $4/mmm$  of  $A^*$  which leaves  $M^*$  invariant is  $K = 4/m$ . This group is generated by the fourfold rotation  $R_1$  and the mirror  $R_2$  perpendicular to the  $z$  axis. Then

$$\begin{array}{ccc} & 0 & -1 & 0 \\ \Gamma_E(R_1) = & 1 & 0 & 0 \\ & 0 & 0 & 1 \\ & 1 & 0 & 0 \\ \Gamma_E(R_2) = & 0 & 1 & 0 \\ & 0 & 0 & -1 \end{array} \quad \begin{array}{ccc} & 0 & -1 \\ \Gamma_I(R_1) = & 1 & 0 \\ & 1 & 0 \\ & 1 & 0 \\ \Gamma_I(R_2) = & 0 & 1 \\ & 0 & 1 \end{array}$$

Hence the arithmetic crystal class of  $\Gamma_E(K)$  is  $P4/m$  and that of  $\Gamma_I(K)$  is  $p4$ . Since  $\sigma^r = 0$  the two-line symbol is

$$P_{p4}^{P4/m}$$

The symbol '1' in the bottom line has been added in order to indicate that  $R_2$  has the identity as internal rotation. Now  $\mathbf{q}_2^*$  is the transform of  $\mathbf{q}_1^*$  under  $R_1$ . Accordingly we can take  $\mathbf{Q}^* = \mathbf{q}_1^*$ . Therefore  $\mathbf{q}_1^* = \mathbf{Q}^*$ ,  $\mathbf{q}_2^* = R_1 \mathbf{Q}^*$  and the one-line symbol is  $P4/m (\alpha, \beta, 0)$ .

## V. Derivation and tables

For the dimensions  $d \leq 3$  the arithmetic crystal classes can be found in IT. To get the  $(3 + d)$ -dimensional holohedral point groups it is sufficient to consider the three-dimensional point groups  $K$  which contain the total inversion  $-1$ . For each of the corresponding arithmetic point groups  $\Gamma_E(K)$ , one considers  $d$ -dimensional arithmetic point groups  $\Gamma_I(K)$  which are homomorphic images of  $K$  (and thus of  $\Gamma_E(K)$ , also). One then takes the corresponding set of pairs  $\{\Gamma_E(R), \Gamma_I(R), R \text{ in } K\}$ . For each pair of this set (20) allows us to derive the restrictions imposed on the admitted matrices  $\sigma^i$ : one then keeps the most general form. The matrices  $\sigma^r$  are representatives of the class of solutions of

$$\sigma \Gamma_E(R) - \Gamma_I(R) \sigma \equiv 0 \quad (\text{modulo integers}), \quad (27)$$

modulo the general solution of (20) considered above. For each group  $\Gamma(K)$  given in terms of one pair  $\Gamma_E(K), \Gamma_I(K)$  one finds in this way one  $\sigma^i$  and one or more matrices  $\sigma^r$ . The equivalent  $\sigma = \sigma^i + \sigma^r$  among these are found using (24). Finally, one eliminates those  $\sigma$  not satisfying the rational independence condition stated in § 2.

As an example we consider the case:  $K = 2/m$ ,  $\Gamma_E(K) = P2/m$  and  $\Gamma_I(K) = P2/m$ . There are two alternative pairings: 2 with 2, or 2 with  $m$ . In the first case

$$\Gamma_E(R_1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \Gamma_I(R_1).$$

The corresponding solution of (20) is

$$\begin{aligned} \sigma' &= \begin{pmatrix} \alpha & \beta & 0 \\ \lambda & \mu & 0 \\ 0 & 0 & \theta \end{pmatrix}. \end{aligned}$$

Putting

$$\begin{aligned} \sigma^r &= \begin{pmatrix} 0 & 0 & \gamma \\ 0 & 0 & \nu \\ \zeta & \eta & 0 \end{pmatrix} \end{aligned}$$

the solutions of (27) satisfy the set of equations

$$2\gamma \equiv 0, \quad 2\nu \equiv 0, \quad 2\zeta \equiv 0, \quad 2\eta \equiv 0 \pmod{\text{integers}}.$$

Since the coefficients of  $\sigma^r$  are determined up to integers (cf. equation 24), there are  $2^4 = 16$  solutions. Applying again (24), one finds that there are four inequivalent solutions to  $\sigma^r$  (see the Appendix):

$$\begin{array}{cccccccccc} 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 \end{array}$$

These give rise to the following four Bravais classes:

$$P_{P2/m}^{P2/m} \quad C_{1P2/m}^{P2/m} \quad C_{2P2/m}^{P2/m} \quad C_{3P2/m}^{P2/m}$$

which can be found in Table 1(c).

Once one has determined all non-equivalent matrices  $\sigma$  for all groups  $\Gamma(K) = \{\Gamma_E(K), \Gamma_I(K)\}$ , one has to eliminate those cases which are not holohedral point groups for the lattices they leave invariant. If one finds for  $\Gamma(K)$  the same (or equivalent)  $\sigma$  as for  $\Gamma(K')$  with  $K$  a subgroup of  $K'$ , then one deletes the first case.

In this way we have determined all  $(3 + d)$ -dimensional Bravais classes for  $d \leq 3$ . They are indicated in Table 1 by their one-line symbol. The corresponding two-line symbol can easily be constructed. The top line designates  $\Gamma_E(K)$ , present in the one-line symbol as well. The bottom line is given in the third column. The prefix is  $P$  for the first Bravais class given  $\Gamma(K)$  and  $\sigma^r = 0$ , it is  $C_1$  for the second, if present, and so on. For  $d = 1$  the prefix is explicitly given with the convention adopted by Janner, Janssen & de Wolff (1979).

In Table 2 one finds how many  $(3 + d)$ -dimensional Bravais classes there are for each of the three-

dimensional crystallographic systems, as far as has been worked out in the present approach.

## VI. Arithmetic crystal classes and superspace groups

The Bravais classes discussed above characterize the lattices appearing in superspace groups which describe the symmetry of incommensurate crystal phases. Each Bravais class corresponds to the arithmetic crystal class of the holohedral point group. The other arithmetic crystal classes can be found as non-equivalent subgroups of the former ones. For these arithmetic crystal classes one can use the same one- or two-line symbol as for the Bravais class. One simply indicates the occurring point group instead of the holohedral one.

As an example consider the Bravais class

$$P2/m(\alpha, \beta, \gamma) = P_{cmm}^{P2/m}.$$

The holohedral point group is of order four and has three subgroups of order two:  $P2(\alpha, \beta, \gamma)$ ,  $Pm(\alpha, \beta, \gamma)$ ,  $P1(\alpha, \beta, \gamma)$ . The last one is the holohedral point group of another Bravais class. Hence the three arithmetic crystal classes belonging to the Bravais class considered are  $P2/m(\alpha, \beta, \gamma)$ ,  $P2(\alpha, \beta, \gamma)$ , and  $Pm(\alpha, \beta, \gamma)$ , or, in their two-line symbols,

$$P_{cmm}^{P2/m} \quad P_{cm}^{P2} \quad P_{cm}^{Pm}$$

We have not undertaken the job of determining all arithmetic point groups having the Bravais classes derived here. Neither did we derive a corresponding full list of superspace groups; this latter would be prohibitively long. In particular cases, however, one can for a given arithmetic point group determine all superspace groups following the algorithm discussed in Janssen, Janner & Ascher (1969) and Fast & Janssen (1968, 1971).

As an example we consider the arithmetic point group  $P432(\alpha, 0, 0)$ , which is a subgroup of the holohedral group  $Pm3m(\alpha, 0, 0)$ . According to Table 1,  $d = 3$ . For a suitable choice of basis the components of the matrix  $\sigma$  are

$$\begin{aligned} \sigma &= \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}. \end{aligned}$$

Using (16) one can determine  $\Gamma_I(4)$  and  $\Gamma_I(3)$  which are equal to  $\Gamma_E(4)$  and  $\Gamma_E(3)$ , respectively. Then one knows the generators  $\Gamma(4)$  and  $\Gamma(3)$  of the point group expressed as  $6 \times 6$ -dimensional matrices. According to Janssen, Janner & Ascher (1969) and Fast & Janssen (1968, 1971) one has to construct

$$\begin{aligned} N_\alpha &= \sum_{k=1}^4 \Gamma(4)^k, \quad N_\beta = \sum_{k=1}^3 \Gamma(3)^k, \\ N_{\alpha\beta} &= 1 + \Gamma(4)\Gamma(3), \quad Z_{\alpha\beta} = N_{\alpha\beta}\Gamma(4), \end{aligned}$$

Table 1. Bravais classes for incommensurate crystal phases with internal dimension  $d = 1, 2$  or  $3$ 

First column: number of the Bravais class; second column: one-line symbol; third column: bottom line for the two-line symbol. The two-line symbol has the first part of the one-line symbol as top line, the given bottom line and a prefix. For  $d = 1$  this prefix is given, for  $d = 2$  and  $3$  it is  $P$  for the first Bravais class with given top and bottom line and  $C_1, C_2, \dots$  for the following ones.

(a) Bravais classes  $d = 1$ 

Triclinic			Orthorhombic			Tetragonal		
1 $P1(\alpha\beta\gamma)$	$\bar{1}$	$P$	9 $Pnmm(00\gamma)$	$11\bar{1}$	$P$	19 $P4/mmm(00\gamma)$	$\bar{1}111$	$P$
Monoclinic			10 $Pnmm(0\frac{1}{2}\gamma)$	$11\bar{1}$	$B$	20 $P4/mmm(\frac{1}{2}\gamma)$	$\bar{1}111$	$W$
2 $P2/m(\alpha\beta 0)$	$\bar{1}1$	$P$	11 $Pnmm(\frac{1}{2}\frac{1}{2}\gamma)$	$11\bar{1}$	$W$	21 $I4/mmm(00\gamma)$	$\bar{1}111$	$P$
3 $P2/m(\alpha\beta\frac{1}{2})$	$\bar{1}1$	$C$	12 $Immm(00\gamma)$	$11\bar{1}$	$P$	Trigonal		
4 $B2/m(\alpha\beta 0)$	$\bar{1}1$	$P$	13 $Cnmm(00\gamma)$	$11\bar{1}$	$P$	22 $R\bar{3}m(00\gamma)$	$\bar{1}1$	$P$
5 $P2/m(00\gamma)$	$\bar{1}1$	$P$	14 $Cnmm(10\gamma)$	$11\bar{1}$	$L$	23 $P\bar{3}1m(\frac{1}{2}\frac{1}{2}\gamma)$	$\bar{1}11$	$R$
6 $P2/m(\frac{1}{2}0\gamma)$	$\bar{1}1$	$A$	15 $Amnm(00\gamma)$	$11\bar{1}$	$P$	Hexagonal		
7 $B2/m(00\gamma)$	$\bar{1}1$	$P$	16 $Amnm(\frac{1}{2}0\gamma)$	$11\bar{1}$	$A$	24 $P6/mmm(00\gamma)$	$\bar{1}111$	$P$
8 $B2/m(0\frac{1}{2}\gamma)$	$\bar{1}1$	$B$	17 $Fmmm(00\gamma)$	$11\bar{1}$	$P$			
			18 $Fmmm(10\gamma)$	$11\bar{1}$	$L$			

(b) Bravais classes  $d = 2$ 

Triclinic			Orthorhombic			Tetragonal		
1 $P1(\alpha\beta\gamma, \lambda\mu\nu)$	$p2$		29 $Pnmm(0\beta 0, 00\nu)$	$p1mm$		57 $P4/m(\alpha\beta 0)$		$p41$
Monoclinic			30 $Pnmm(\frac{1}{2}\beta 0, 00\nu)$	$p1mm$		58 $P4/m(\alpha\beta\frac{1}{2})$		$p41$
2 $P2/m(\alpha\beta 0, \lambda\mu 0)$	$p21$		31 $Pnmm(0\beta\frac{1}{2}, 00\nu)$	$p1mm$		59 $I4/m(\alpha\beta 0)$		$p41$
3 $P2/m(\alpha\beta\frac{1}{2}, \lambda\mu 0)$	$p21$		32 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, 00\nu)$	$p1mm$		60 $P4/mmm(00\gamma, 00\nu)$		$p1211$
4 $B2/m(\alpha\beta 0, \lambda\mu 0)$	$p21$		33 $Pnmm(\frac{1}{2}\beta 0, \frac{1}{2}0\nu)$	$p1mm$		61 $P4/mmm(\frac{1}{2}\frac{1}{2}\gamma, 00\nu)$		$p1211$
5 $P2/m(00\gamma, 00\nu)$	$p12$		34 $Pnmm(\frac{1}{2}\beta 0, 0\frac{1}{2}\nu)$	$p1mm$		62 $I4/mmm(00\gamma, 00\nu)$		$p1211$
6 $P2/m(\frac{1}{2}0\gamma, 00\nu)$	$p12$		35 $Pnmm(0\beta\frac{1}{2}, 0\frac{1}{2}\nu)$	$p1mm$		63 $P4/mmm(\alpha 0 0)$		$p41mm$
7 $P2/m(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu)$	$p12$		36 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}0\nu)$	$p1mm$		64 $P4/mmm(\alpha\frac{1}{2} 0)$		$p41mm$
8 $B2/m(00\gamma, 00\nu)$	$p12$		37 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, 0\frac{1}{2}\nu)$	$p1mm$		65 $P4/mmm(\alpha 0\frac{1}{2})$		$p41mm$
9 $B2/m(0\frac{1}{2}\gamma, 00\nu)$	$p12$		38 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}\frac{1}{2}\nu)$	$p1mm$		66 $P4/mmm(\alpha\frac{1}{2}\frac{1}{2})$		$p41mm$
10 $P2/m(\alpha\beta 0, 00\nu)$	$pmm$		39 $Immm(0\beta 0, 00\nu)$	$p1mm$		67 $I4/m\bar{2}m(\alpha 0 0)$		$p41m\bar{2}m$
11 $P2/m(\alpha\beta\frac{1}{2}, 00\nu)$	$pmm$		40 $Cnmm(0\beta 0, 00\nu)$	$p1mm$		68 $P4/m\bar{2}m(\alpha\alpha 0)$		$p41m\bar{2}m$
12 $P2/m(\alpha\beta 0, \frac{1}{2}0\nu)$	$pmm$		41 $Cnmm(0\beta\frac{1}{2}, 00\nu)$	$p1mm$		69 $P4/m\bar{2}m(\alpha\alpha\frac{1}{2})$		$p41m\bar{2}m$
13 $P2/m(\alpha\beta\frac{1}{2}, \frac{1}{2}0\nu)$	$pmm$		42 $Cnmm(0\beta 0, 10\nu)$	$p1mm$		70 $I4/m\bar{2}m(\alpha\alpha 0)$		$p41m\bar{2}m$
14 $B2/m(\alpha\beta 0, 00\nu)$	$pmm$		43 $Cnmm(0\beta\frac{1}{2}, 10\nu)$	$p1mm$		71 $I4/m\bar{2}m(\alpha\alpha 1)$		$p41m\bar{2}m$
15 $B2/m(\alpha\beta 0, \frac{1}{2}\nu)$	$pmm$		44 $Amnm(0\beta 0, 00\nu)$	$p1mm$		Trigonal		
16 $P2/m(\alpha\beta\gamma)$	$cm$		45 $Amnm(\frac{1}{2}\beta 0, 00\nu)$	$p1mm$		72 $P\bar{3}(a\beta\frac{1}{2})$		$p6$
17 $B2/m(\alpha\beta\gamma)$	$cm$		46 $Amnm(\frac{1}{2}\beta 0, \frac{1}{2}\nu)$	$p1mm$		73 $R\bar{3}(a\beta 0)$		$p6$
Orthorhombic			47 $Fmmm(0\beta 0, 00\nu)$	$p1mm$		74 $P\bar{3}1m(\frac{1}{2}\frac{1}{2}\gamma, 00\nu)$		$p211$
18 $Pnmm(00\gamma, 00\nu)$	$p112$		48 $Fmmm(1\beta 0, 00\nu)$	$p1mm$		75 $R\bar{3}m(00\gamma, 00\nu)$		$p21$
19 $Pnmm(0\frac{1}{2}\gamma, 00\nu)$	$p112$		49 $Fmmm(1\beta 0, 10\nu)$	$p1mm$		76 $P\bar{3}1m(\alpha\alpha\frac{1}{2})$		$p61m$
20 $Pnmm(\frac{1}{2}\frac{1}{2}\gamma, 00\nu)$	$p112$		50 $Pnmm(0\beta\gamma)$	$c1mm$		77 $R\bar{3}m(\alpha\alpha 0)$		$p6\bar{m}$
21 $Pnmm(\frac{1}{2}\gamma, 0\frac{1}{2}\nu)$	$p112$		51 $Pnmm(\frac{1}{2}\beta\gamma)$	$c1mm$		78 $P\bar{3}1m(\alpha 0\frac{1}{2})$		$p6m1$
22 $Immm(00\gamma, 00\nu)$	$p112$		52 $Immm(0\beta\gamma)$	$c1mm$		79 $R\bar{3}m(\alpha 0 0)$		$p6m$
23 $Cnmm(00\gamma, 00\nu)$	$p112$		53 $Cnmm(0\beta\gamma)$	$c1mm$		Hexagonal		
24 $Cnmm(10\gamma, 00\nu)$	$p112$		54 $Amnm(0\beta\gamma)$	$c1mm$		80 $P6/m(\alpha\beta 0)$		$p61$
25 $Amnm(00\gamma, 00\nu)$	$p112$		55 $Amnm(\frac{1}{2}\beta\gamma)$	$c1mm$		81 $P6/mmm(00\gamma, 00\nu)$		$p1211$
26 $Amnm(\frac{1}{2}0\gamma, 00\nu)$	$p112$		56 $Fmmm(0\beta\gamma)$	$c1mm$		82 $P6/mmm(\alpha 0 0)$		$p61m\bar{2}m$
27 $Fmmm(00\gamma, 00\nu)$	$p112$					83 $P6/mmm(\alpha\alpha 0)$		$p61m\bar{2}m$
28 $Fmmm(10\gamma, 00\nu)$	$p112$							

(c) Bravais classes  $d = 3$ 

Triclinic			Orthorhombic			Tetragonal		
1 $P1(\alpha\beta\gamma, \lambda\mu\nu, \zeta\eta\theta)$	$P\bar{1}$		30 $Pnmm(00\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		60 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, 0\frac{1}{2}\nu, \frac{1}{2}\theta)$		$P1m/2$
Monoclinic			31 $Pnmm(0\frac{1}{2}\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		61 $Immm(0\beta 0, 00\nu, 00\theta)$		$P1m/2$
2 $P2/m(\alpha\beta 0, \lambda\mu 0, \zeta\eta\theta)$	$P\bar{1}1$		32 $Pnmm(\frac{1}{2}\frac{1}{2}\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		62 $Cnmm(0\beta 0, 00\nu, 00\theta)$		$P1m/2$
3 $P2/m(\alpha\beta\frac{1}{2}, \lambda\mu 0, \zeta\eta\theta)$	$P\bar{1}1$		33 $Pnmm(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, 00\theta)$	$P11\bar{1}$		63 $Cnmm(0\beta\frac{1}{2}, 00\nu, 00\theta)$		$P1m/2$
4 $B2/m(\alpha\beta 0, \lambda\mu 0, \zeta\eta\theta)$	$P\bar{1}1$		34 $Immm(00\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		64 $Cnmm(0\beta 0, 10\nu, 00\theta)$		$P1m/2$
5 $P2/m(00\gamma, 00\nu, 00\theta)$	$P\bar{1}1$		35 $Cnmm(00\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		65 $Cnmm(0\beta\frac{1}{2}, 10\nu, 00\theta)$		$P1m/2$
6 $P2/m(\frac{1}{2}0\gamma, 00\nu, 00\theta)$	$P\bar{1}1$		36 $Cnmm(10\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		66 $Bnmm(0\beta 0, 00\nu, 00\theta)$		$P1m/2$
7 $P2/m(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, 00\theta)$	$P\bar{1}1$		37 $Amnm(00\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		67 $Bnmm(1\beta 0, 00\nu, 00\theta)$		$P1m/2$
8 $P2/m(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, \frac{1}{2}\theta)$	$P\bar{1}1$		38 $Amnm(\frac{1}{2}0\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		68 $Bnmm(0\beta 0, \frac{1}{2}\nu, 00\theta)$		$P1m/2$
9 $B2/m(00\gamma, 00\nu, 00\theta)$	$P\bar{1}1$		39 $Fmmm(00\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		69 $Bnmm(1\beta 0, \frac{1}{2}\nu, 00\theta)$		$P1m/2$
10 $B2/m(0\frac{1}{2}\gamma, 00\nu, 00\theta)$	$P\bar{1}1$		40 $Fmmm(10\gamma, 00\nu, 00\theta)$	$P11\bar{1}$		70 $Amnm(0\beta 0, 00\nu, 00\theta)$		$P1m/2$
11 $P2/m(\alpha\beta 0, \lambda\mu 0, 00\theta)$	$P2/m$		41 $Pnmm(0\beta 0, 00\nu, 00\theta)$	$P1m/2$		71 $Amnm(\frac{1}{2}\beta 0, 00\nu, 00\theta)$		$P1m/2$
12 $P2/m(\alpha\beta\frac{1}{2}, \lambda\mu 0, 00\theta)$	$P2/m$		42 $Pnmm(\frac{1}{2}\beta 0, 00\nu, 00\theta)$	$P1m/2$		72 $Amnm(0\beta 0, \frac{1}{2}\nu, 00\theta)$		$P1m/2$
13 $P2/m(\alpha\beta 0, \lambda\mu 0, \frac{1}{2}\theta)$	$P2/m$		43 $Pnmm(0\beta\frac{1}{2}, 00\nu, 00\theta)$	$P1m/2$		73 $Amnm(\frac{1}{2}\beta 0, \frac{1}{2}\nu, 00\theta)$		$P1m/2$
14 $P2/m(\alpha\beta\frac{1}{2}, \lambda\mu 0, \frac{1}{2}\theta)$	$P2/m$		44 $Pnmm(0\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		74 $Fmnm(0\beta 0, 00\nu, 00\theta)$		$P1m/2$
15 $B2/m(\alpha\beta 0, \lambda\mu 0, 00\theta)$	$P2/m$		45 $Pnmm(0\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		75 $Fmnm(1\beta 0, 00\nu, 00\theta)$		$P1m/2$
16 $B2/m(\alpha\beta 0, \lambda\mu 0, \frac{1}{2}\theta)$	$P2/m$		46 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, 00\nu, 00\theta)$	$P1m/2$		76 $Fmnm(0\beta 0, 10\nu, 00\theta)$		$P1m/2$
17 $P2/m(\alpha\beta 0, \lambda\mu\nu)$	$A2/m$		47 $Pnmm(\frac{1}{2}\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		77 $Fmnm(1\beta 0, 10\nu, 00\theta)$		$P1m/2$
18 $P2/m(\alpha\beta\frac{1}{2}, \lambda\mu\nu)$	$A2/m$		48 $Pnmm(\frac{1}{2}\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		78 $Pnmm(00\gamma, 0\mu\nu)$		$A1m/2$
19 $B2/m(\alpha\beta 0, \lambda\mu\nu)$	$A2/m$		49 $Pnmm(0\beta\frac{1}{2}, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		79 $Pnmm(\frac{1}{2}\gamma, 0\mu\nu)$		$A1m/2$
20 $P2/m(\alpha\beta 0, 00\nu, 00\theta)$	$Pm/2$		50 $Pnmm(0\beta\frac{1}{2}, 0\frac{1}{2}\nu, 00\theta)$	$P1m/2$		80 $Pnmm(0\frac{1}{2}\gamma, 0\mu\nu)$		$A1m/2$
21 $P2/m(\alpha\beta\frac{1}{2}, 00\nu, 00\theta)$	$Pm/2$		51 $Pnmm(0\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		81 $Pnmm(00\gamma, \frac{1}{2}\mu\nu)$		$A1m/2$
22 $P2/m(\alpha\beta 0, \frac{1}{2}\nu, 00\theta)$	$Pm/2$		52 $Pnmm(0\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		82 $Pnmm(\frac{1}{2}\frac{1}{2}\gamma, 0\mu\nu)$		$A1m/2$
23 $P2/m(\alpha\beta\frac{1}{2}, \frac{1}{2}\nu, 00\theta)$	$Pm/2$		53 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		83 $Pnmm(\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$		$A1m/2$
24 $B2/m(\alpha\beta 0, 00\nu, 00\theta)$	$Pm/2$		54 $Pnmm(\frac{1}{2}\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		84 $Pnmm(0\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$		$A1m/2$
25 $B2/m(\alpha\beta 0, \frac{1}{2}\nu, 00\theta)$	$Pm/2$		55 $Pnmm(\frac{1}{2}\beta 0, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		85 $Pnmm(\frac{1}{2}\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$		$A1m/2$
26 $P2/m(\alpha\beta\gamma, 00\nu)$	$Cm/2$		56 $Pnmm(\frac{1}{2}\beta 0, 0\frac{1}{2}\nu, \frac{1}{2}\theta)$	$P1m/2$		86 $Immm(00\gamma, 0\mu\nu)$		$A1m/2$
27 $P2/m(\alpha\beta\gamma, \frac{1}{2}\nu)$	$Cm/2$		57 $Pnmm(0\beta\frac{1}{2}, 0\frac{1}{2}\nu, \frac{1}{2}\theta)$	$P1m/2$		87 $Cnmm(00\gamma, 0\mu\nu)$		$A1m/2$
28 $B2/m(\alpha\beta\gamma, 00\nu)$	$Cm/2$		58 $Pnmm(0\beta\frac{1}{2}, 0\frac{1}{2}\nu, \frac{1}{2}\theta)$	$P1m/2$		88 $Cnmm(10\gamma, 0\mu\nu)$		$A1m/2$
29 $B2/m(\alpha\beta\gamma, 0\frac{1}{2}\nu)$	$Cm/2$		59 $Pnmm(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}\nu, 00\theta)$	$P1m/2$		89 $Bnmm(00\gamma, 0\mu\nu)$		$A1m/2$
						90 $Bnmm(0\frac{1}{2}\gamma, 0\mu\nu)$		$A1m/2$





These superspace groups can be indicated by the following symbols:

- (1)  $P432(\alpha,0,0)$  (6)  $P4_232(\alpha,0,0)(4_1,0,0)$   
 (2)  $P4_132(\alpha,0,0)$  (7)  $P432(\alpha,0,0)(4_2,0,0)$   
 (3)  $P4_232(\alpha,0,0)$  (8)  $P4_132(\alpha,0,0)(4_2,0,0)$   
 (4)  $P432(\alpha,0,0)(4_1,0,0)$  (9)  $P4_232(\alpha,0,0)(4_2,0,0)$   
 (5)  $P4_132(\alpha,0,0)(4_1,0,0)$

The last parentheses in the symbol contain indications concerning the internal components of the non-primitive translations associated with each of the three generators.

## APPENDIX

### The non-equivalent solutions $\sigma^r$

In § 5 one has seen that there are 16 solutions for the matrix  $\sigma^r$  if  $\Gamma_E(K) = P2/m = \Gamma_I(K)$ . Since solutions can be added to give new solutions and the matrices are only determined up to integers, one can denote them by binary numbers. The four fundamental solutions can be written as:

$$\begin{array}{l} 0000 = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad 0100 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ 0010 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}, \quad 0001 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix} \end{array}$$

Then the 16 solutions are 0000, 1000, 0100, 1100, ..., 1111. To determine the equivalent ones one has to apply (24) with  $S$  and  $T$  such that the form of  $\sigma^i$  remains the same. One can formulate this in another way: the matrices  $S$  and  $T$  have to leave  $\Gamma_E(K)$  and  $\Gamma_I(K)$ , respectively, invariant [using (16)]. One may take  $S$  and  $T$  matrices from the group generated by

$$M_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Table 3. Transformation of fundamental solutions for  $K_E = K_I = 2/m$

$\sigma^r$  to which  $\sigma$  is mapped by  $S$  and  $T$  ( $E$  indicates the unit matrix).

$T$	$S$	$\sigma$ :	1000	0100	0010	0001
$E$	$M_1$		1000	0100	0001	0010
$E$	$M_2$		1000	0100	0011	0001
$M_1$	$E$		0100	1000	0010	0001
$M_2$	$E$		1000	1100	0010	0001

Table 4. Equivalence relation between the 16 solutions for  $K_E = K_I = 2/m$ .

	0000	1000	0100	1100	0010	1010	0110	1110	0001	1001	0101	1101	0011	1011	0111	1111
0000	A															
1000		B	x													
0100			x	B	x											
1100				x	B											
0010						C			x				x			
1010							D	x		x				x		
0110								x	D	x			x			x
1110									x	D			x			x
0001					x					C						
1001						x					D	x				
0101							x				x	D	x			
1101								x				x	D			
0011					x									C		
1011						x									D	x
0111							x								x	D
1111								x								x

It is easily verified that  $M_1, M_2$  leave both point groups  $\Gamma_E(K)$  and  $\Gamma_I(K)$  invariant. Application of (24) then maps each  $\sigma^r$  to a  $\sigma^{r'}$ , the result of which is given in Table 3 for the four basic solutions. By linearity then the action of  $M_1$  and  $M_2$  on all 16 solutions is determined. In Table 4 is indicated to which solution each of these 16 solutions is mapped by the transformations indicated in Table 3. It is then easily seen what are the equivalence classes. On the diagonal of Table 4 it is indicated by a letter to which class a solution belongs. Taking one representative from each class one obtains the four non-equivalent solutions.

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