This set of vectors is a vector module M^*. The vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ form a basis of the reciprocal lattice Λ^* of the basic structure and $\mathbf{q}$ is the modulation wavevector. The choice of the basis of Λ^* has the usual freedom, the wavevector $\mathbf{q}$ is only determined up to a sign and up to a reciprocal-lattice vector of the basic structure.

A vector module M^* has point-group symmetry K, which is the subgroup of all elements R of $O(3)$ leaving it invariant.

In the case of an incommensurate one-dimensional modulation, M^* is generated by the lattice Λ^* of main reflections and the modulation wavevector $\mathbf{q}$. It then follows that K is characterized by the following properties:

(1) It leaves Λ^* invariant. (Only in this way are main reflections transformed into main reflections and satellites into satellites.)

(2) Any element R of K then transforms $\mathbf{q}$ into $\pm\mathbf{q}$ (modulo reciprocal-lattice vectors of Λ^*).

An element R of K then transforms the basic vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$, $\mathbf{q}$ into ones of the form (9.8.1.15). If one denotes, as in (9.8.1.2), $\mathbf{q}$ by $\mathbf{a}_4^*$, this implies

$$R\mathbf{a}_i^* = \sum_{j=1}^{4} \Gamma^*(R)_{ji}\mathbf{a}_j^*, \quad i = 1, \ldots, 4, \tag{9.8.1.16}$$

with $\Gamma^*(R)$ a 4×4 matrix with integral entries. In the case of an incommensurate modulated crystal structure, only two vectors with the same length as $\mathbf{q}$ are $\mathbf{q}$ and $-\mathbf{q}$. As Λ^* is left invariant, it follows that for a one-dimensionally modulated structure $\Gamma^*(R)$ has the form

$$\Gamma^*(R) = \begin{pmatrix} \Gamma_E^*(R) & \Gamma_M^*(R) \\ 0 & \varepsilon(R) \end{pmatrix}, \quad \text{where } \varepsilon(R) = \pm 1. \tag{9.8.1.17}$$

This matrix represents the orthogonal transformation R when referred to the basis vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3, 4)$ of the vector module M^*. As in the case of lattices, two vector modules of modulated crystals are equivalent if they have bases (*i.e.* a basis for the reciprocal lattice Λ^* of the basic structure together with a modulation wavevector $\mathbf{q}$) such that the set of matrices $\Gamma^*(K)$ representing their symmetry is the same for both vector modules. Equivalent vector modules form a *Bravais class*.

Again, as in the case of three-dimensional lattices, it is sometimes convenient to consider a vector module that includes as subset the one spanned by all diffraction spots as in (9.8.1.15). Within such a larger vector module, the actual diffraction peaks then obey *centring conditions*. For a vector module associated with a modulated structure, centring may involve main reflections (the basic structure then has a centred lattice), or satellites, or both. For example, if in a structure with primitive orthorhombic basic structure the modulation wavevector is given by $\alpha\mathbf{a}_1^* + \frac{1}{2}\mathbf{a}_2^*$, one may describe the diffraction spots by means of the non-primitive lattice basis $\mathbf{a}_1^*, \frac{1}{2}\mathbf{a}_2^*, \mathbf{a}_3^*$ and by the modulation wavevector $\alpha\mathbf{a}_1^*$.

Crystallographic point groups are denoted generally by the same letter K.

9.8.1.4.2. *Description in four dimensions*

The matrices $\Gamma^*(R)$ form a faithful integral representation of the three-dimensional point group K. It is also possible to consider them as four-dimensional orthogonal transformations leaving a lattice with basis vectors (9.8.1.14) invariant. Indeed, one can consider the vectors (9.8.1.15) as *projections* of four-dimensional lattice vectors $H_s = (\mathbf{H}, H_I)$, which can be written as

$$H_s = \sum_{i=1}^{4} h_i a_{si}^*, \tag{9.8.1.18}$$

where [*cf.* (9.8.1.14)] m has now been replaced by h_4 and

$$a_{si}^* = (\mathbf{a}_i^*, 0), \quad i = 1, 2, 3; \quad a_{s4}^* = (\mathbf{q}, 1). \tag{9.8.1.19}$$

As will be explained in Section 9.8.4, these vectors span the four-dimensional reciprocal lattice for a periodic structure having as three-dimensional intersection (say defined by the hyperplane $t = 0$) the modulated crystal structure (a specific example has been given in Subsection 9.8.1.3). In direct space, the point group K_s in four dimensions with elements R_s of $O(4)$ then acts on the corresponding dual basis vectors (9.8.1.11) of the four-dimensional *direct lattice* as

$$R_s a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj} \quad (i = 1, 2, 3, 4), \tag{9.8.1.20a}$$

where $\Gamma(R)$ is the transpose of the matrix $\Gamma^*(R^{-1})$ appearing in (9.8.1.17) and therefore for incommensurate one-dimensionally modulated structures it has the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \varepsilon(R) \end{pmatrix}. \tag{9.8.1.20b}$$

9.8.1.4.3. *Four-dimensional crystallography*

Let us summarize the results obtained in the previous paragraph. The matrices $\Gamma(R)$ form a faithful integral representation of the three-dimensional point group K with a four-dimensional carrier space V_s. It is a reducible representation having as invariant subspaces the physical three-dimensional space, denoted by V (or sometimes also by V_E), and the additional one-dimensional space, denoted by V_I. In V, the four-dimensional point-group transformation acts as R (sometimes also denoted by R_E), in V_I it acts as one of the two one-dimensional point-group transformations: the identity or the inversion. Therefore, the space V_s can be made Euclidean with $\Gamma(R)$ defining a four-dimensional point-group transformation R_s, which is an element of a crystallographic subgroup K_s of $O(4)$. The four-dimensional point-group transformations are of the form (R, ε), with $\varepsilon = \pm 1$ and they act on the four-dimensional lattice basis as

$$(R, \varepsilon)a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj}, \quad i = 1, \ldots, 4, \tag{9.8.1.21}$$

where ε stands for $\varepsilon(R)$ as in (9.8.1.20*b*). So the point-group symmetry operations are crystallographic and given by pairs of a three-dimensional crystallographic point-group transformation and a one-dimensional $\varepsilon = \pm 1$, respectively. The case $\varepsilon = -1$ corresponds to an *inversion of the phase of the modulation function*.

As in the three-dimensional case, one can define equivalence classes among those four-dimensional point groups.

Two point groups K_s and K_s' belong to the same *geometric crystal class* if their three-dimensional (external) parts (forming the point group K_E and K_E', respectively) are in the same three-dimensional crystal class [*i.e.* are conjugated subgroups of $O(3)$] and their one-dimensional internal parts (forming the point groups K_I and K_I', respectively) are equal. The latter condition implies that corresponding point-group elements have the same value of ε.

Such a geometric crystal class can then be denoted by the symbol of the three-dimensional crystal class together with the values of ε that correspond to the generators.

Also, the notion of *arithmetic equivalence* can be generalized to these four-dimensional point groups, as they admit the same faithful integral representation $\Gamma(K)$ given above. This means

that two such groups are arithmetically equivalent if there is a basis transformation for the reciprocal-vector module, which transforms main reflections into main reflections and satellites into satellites and which transforms one of the matrix groups into the other. The arithmetic classes are determined by the arithmetic equivalence class of the three-dimensional group K_E [*i.e.* by $\Gamma_E(K)$] and by the components of the modulation wavevector with respect to the corresponding reciprocal-lattice basis. This is because the elements ε are fixed by the relation

$$R\mathbf{q} \equiv \varepsilon\mathbf{q} \text{ (modulo reciprocal-lattice vectors of the basic structure).} \qquad (9.8.1.22)$$

Note that these $(3+1)$-dimensional equivalence classes are not simply those one obtains in four-dimensional crystallography, as the relation between the higher-dimensional space V_s and the three-dimensional physical space V plays a fundamental role.

The embedded structures in four dimensions have lattice periodicity. So the symmetry groups are four-dimensional space groups, called *superspace groups*. The new name has been introduced because of the privileged role played by the three-dimensional subspace V. A superspace-group element g_s consists of a point-group transformation (R, ε) and a translation $(\mathbf{v}, \Delta)$. The action of such an element on the four-dimensional space is then given by

$$g_s r_s = \{(R, \varepsilon)|(\mathbf{v}, \Delta)\}(\mathbf{r}, t) = (R\mathbf{r} + \mathbf{v}, \varepsilon t + \Delta). \qquad (9.8.1.23)$$

It is important to realize that a superspace-group symmetry of an embedded crystal induces three-dimensional transformations leaving the original modulated structure invariant. Corresponding to (9.8.1.23), one obtains the following relations [*cf.* (9.8.1.13)]:

$$\boldsymbol{u}_{j'}[\mathbf{q}\cdot(\mathbf{n}' + \mathbf{r}_{j'})] = R\mathbf{u}_j[\mathbf{q}\cdot(\mathbf{n} + \mathbf{r}_j) - \varepsilon\Delta] \qquad (9.8.1.24)$$

with

$$\mathbf{n}' + \mathbf{r}_{j'} = R(\mathbf{n} + \mathbf{r}_j) + \mathbf{v}.$$

These are purely three-dimensional symmetry relations, but of course not Euclidean ones.

In three-dimensional Euclidean space, the types of space-group transformation are translations, rotations, rotoinversions, reflections, central inversion, screw rotations, and glide planes. Only the latter two transformations have intrinsic non-primitive translations. For superspace groups, the types of transformation are determined by the point-group transformations. By an appropriate choice of the basis in V_s, each of the latter can be brought into the form

$$\begin{pmatrix} \cos\varphi & -\sin\varphi & 0 & 0 \\ \sin\varphi & \cos\varphi & 0 & 0 \\ 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}; \quad \varepsilon, \delta = \pm 1. \qquad (9.8.1.25)$$

By a choice of origin, each translational part can be reduced to its intrinsic part, which in combination with the point-group element (R, ε) gives one of the transformations in V indicated above together with the inversion, or the identity, or a shift in V_I. So, for phase inversion (when $\varepsilon = -1$), the intrinsic shift in V_I vanishes. When $\varepsilon = +1$, the intrinsic shift in V_I is given by τ. It will be shown in Subsection 9.8.3.3 that the value of τ is one of

$$0, \frac{1}{2}, \frac{\pm 1}{3}, \frac{\pm 1}{4}, \frac{\pm 1}{6}. \qquad (9.8.1.26)$$

Therefore, a superspace-group element can be denoted by a symbol that consists of a symbol for the three-dimensional part following the conventions given in Volume A of *International Tables for Crystallography*, a symbol that determines ε, and one for the corresponding intrinsic internal translation τ.

9.8.1.4.4. *Generalized nomenclature*

In Section 9.8.4, the theory is extended to structures containing d modulations, with $d \geq 1$. In this case, each point-group transformation in internal space is given by R_I and the associated internal translation by the (d-dimensional) vector $\mathbf{v}_I$. Thus,

$$g_s = \{(R, R_I)|(\mathbf{v}, \mathbf{v}_I)\}.$$

The transformations R and R_I are represented by the matrices $\Gamma_E(R)$ and $\Gamma_I(R)$, respectively. In the following discussion, this nomenclature (but with v_I rather than $\mathbf{v}_I$) is sometimes also applied for the $(3+1)$-dimensional case. The usual formulae are obtained by replacing R_I by ε and v_I by Δ.

9.8.1.4.5. *Four-dimensional space groups*

Four-dimensional space groups were obtained in the $(3+1)$-reducible case by Fast & Janssen (1969) and in the general case by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978). The groups were determined on the basis of algorithms developed by Zassenhaus (1948), Janssen, Janner & Ascher (1969), Brown (1969), and Fast & Janssen (1971). In the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, quoted above, a mathematical characterization of the basic crystallographic concepts is given together with corresponding tables for the dimensions one, two, three, and four. One finds there, in particular, a full list of four–dimensional space groups. The list by Fast & Janssen is restricted to space groups with $(3+1)$-reducible point groups. The four-dimensional groups in the work of Brown *et al.* are labelled by numbers. For these same groups, alternative symbols have been developed by Weigel, Phan, Veysseyre and Grebille generalizing the principles of the notation adopted by *International Tables for Crystallography*, Volume A, for the three-dimensional space groups (Weigel, Phan & Veysseyre, 1987; Veysseyre & Weigel, 1989; Grebille, Weigel, Veysseyre & Phan, 1990).

The difference in the listing of four-dimensional crystallographic groups one finds in Brown *et al.* and in Weigel *et al.* with respect to that in the present tables is not simply a matter of notation. In the first place, here only those groups appear that can occur as symmetry groups of one-dimensional incommensurate modulated phases (there are 371 such space groups). Furthermore, as already mentioned, a finer equivalence relation has been considered that reflects the freedom one has in embedding a three-dimensional modulated structure in a four-dimensional Euclidean space. Instead of 371, one then obtains 775 inequivalent groups for which the name superspace group has been introduced. A $(3+1)$-dimensional superspace group is thus a four-dimensional space group having some additional properties. In Section 9.8.4, the precise definitions are given.

In the commensurate one-dimensionally modulated case, 3833 four-dimensional space groups may occur, out of which 320 already belong to the previous 371. The corresponding additional $(3+1)$-dimensional superspace groups are also present in the listing by Fast & Janssen (1969) and have been considered again (and applied to structure determination) by van Smaalen (1987). The Bravais classes for the commensurate $(3+1)$-dimensional case are given in Table 9.8.3.2(*b*).

The relation between modulated crystals and the superspace groups is treated in a textbook by Opechowski (1986). That between the superspace-group symbols of the present tables and those of Weigel *et al.* is discussed in Grebille *et al.* (1990).