International Tables for Crystallography (2006). Vol. C, Section 9.8.4.3.3, p. 940.

(9.8.4.13). It is then faithfully represented by integral matrices that are of the form indicated in (9.8.4.17) and (9.8.4.18).

9.8.4.3.2. *Crystallographic systems*

Definition 5. A *crystallographic system* is a set of lattices having geometrically equivalent holohedral point groups.

In this way, a given holohedral point group (and even each crystallographic point group) belongs to exactly one system. Two lattices belong to the same system if there are orthonormal bases in V and in V_I, respectively, such that the holohedral point groups of the two lattices are represented by the same set of matrices.

9.8.4.3.3. *Bravais classes*

Definition 6. Two lattices belong to the same *Bravais class* if their holohedral point groups are arithmetically equivalent.

This means that each of them admits a lattice basis of standard form such that their holohedral point group is represented by the same set of integral matrices.

9.8.4.4. *Superspace groups*

9.8.4.4.1. *Symmetry elements*

The elements of a $(3+d)$-dimensional superspace group are pairs of Euclidean transformations in 3 and d dimensions, respectively:

$$g_s = (\{R|\mathbf{v}\}, \{R_I|\mathbf{v}_I\}) \in E(3) \times E(d), \qquad (9.8.4.28)$$

i.e. are elements of the direct product of the corresponding Euclidean groups. The elements $\{R|\mathbf{v}\}$ form a three-dimensional space group, but the same does not hold for the elements $\{R_I|\mathbf{v}_I\}$ of $E(d)$. This is because the internal translations $\mathbf{v}_I$ also contain the 'compensating' transformations associated with the corresponding translation $\mathbf{v}$ in V [see (9.8.4.32)]. In other words, a basis of the lattice Σ does not simply split into one basis for V and one for V_I.

As for elements of a three-dimensional space group, the translational component $\upsilon_s = (\mathbf{v}, \mathbf{v}_I)$ of the element g_s can be decomposed into an intrinsic part υ_s^o and an origin-dependent part υ_s^a:

$$(\boldsymbol{\upsilon}, \boldsymbol{\upsilon}_I) = (\mathbf{v}^o, \mathbf{v}_I^o) + (\mathbf{v}^a, \mathbf{v}_I^a),$$

with

$$(\mathbf{v}^o, \mathbf{v}_I^o) = \frac{1}{n}\sum_{m=1}^{n} (R^m\mathbf{v}, R_I^m\mathbf{v}_I), \qquad (9.8.4.29)$$

where n denotes the order of the element R. In particular, for $d=1$ the intrinsic part $\mathbf{v}_I^o$ of $\mathbf{v}_I$ is equal to $\mathbf{v}_I$ if $R_I = \varepsilon = +1$ and vanishes if $\varepsilon = -1$. The latter means that for $d=1$ there is always an origin in the internal space such that the internal shift $\mathbf{v}_I$ can be chosen to be zero for an element with $\varepsilon = -1$.

The internal part of the intrinsic translation can itself be decomposed into two parts. One part stems from the presence of a translation in the external space. The lattice of the $(3+d)$-dimensional space group has basis vectors

$$(\mathbf{a}_i, \mathbf{a}_{Ii}), (0, \mathbf{d}_j), \quad i = 1, 2, 3, \quad j = 1, \ldots, d. \qquad (9.8.4.30)$$

The internal part of the first three basis vectors is

$$\mathbf{a}_{Ii} = -\Delta\mathbf{a}_i = -\sum_{j=1}^{d} \sigma_{ji}\mathbf{d}_j \qquad (9.8.4.31)$$

according to equation (9.8.4.20). The three-dimensional translation $\mathbf{v} = \sum_i \upsilon_i \mathbf{a}_i$ then entails a d-dimensional translation $-\Delta\mathbf{v}$ in V_I given by

$$\Delta\mathbf{v} = \Delta\left(\sum_{i=1}^{3} \upsilon_i \mathbf{a}_i\right) = \sum_{i=1}^{3} \upsilon_i \Delta\mathbf{a}_i. \qquad (9.8.4.32)$$

These are the so-called compensating translations. Hence, the internal translation $\mathbf{v}_I$ can be decomposed as

$$\mathbf{v}_I = -\Delta\mathbf{v} + \boldsymbol{\delta}, \qquad (9.8.4.33)$$

where $\boldsymbol{\delta} = \sum_{j=1}^{d} \upsilon_{3+j}\mathbf{d}_j$.

This decomposition, however, does still depend on the origin. Consider the case $d=1$. Then an origin shift $\mathbf{s}$ in the three-dimensional space changes the translation $\mathbf{v}$ to $\mathbf{v} + (1-R)\mathbf{s}$ and its internal part $-\Delta\mathbf{v} = -\mathbf{q}\cdot\mathbf{v}$ to $-\mathbf{q}\cdot\mathbf{v} - \mathbf{q}\cdot(1-R)\mathbf{s}$. This implies that for the case that $\varepsilon = 1$ the part δ changes to $\delta + \mathbf{q}\cdot(1-R)\mathbf{s} = \delta + \mathbf{q}^r\cdot(1-R)\mathbf{s}$, because $\mathbf{q}^i$ is invariant under R. Therefore, δ changes, in general. The internal translation

$$\tau = \delta - \mathbf{q}^r \cdot \mathbf{v}, \qquad (9.8.4.34)$$

however, is invariant under an origin shift in V.

Definition 7. *Equivalent superspace groups*. Two superspace groups are equivalent if they are isomorphic and have point groups that are arithmetically equivalent.

Another definition leading to the same partition of equivalent superspace groups considers equivalency with respect to affine transformations among bases of standard form.

This means that two equivalent superspace groups admit standard bases such that the two space groups are represented by the same set of $(4+d)$-dimensional affine transformation matrices. We recall that an n-dimensional Euclidean transformation $g_s = \{R_s|v_s\}$ if referred to a basis of the space can be represented isomorphically by an $(n+1)$-dimensional matrix, of the form

$$A(g_s) = \begin{pmatrix} R_s & v_s \\ 0 & 1 \end{pmatrix} \qquad (9.8.4.35)$$

with R_s an $n \times n$ matrix and v_s an n-dimensional column matrix, all with real entries.

9.8.4.4.2. *Equivalent positions and modulation relations*

A $(3+d)$-dimensional space group that leaves a function invariant maps points in $(3+d)$-space to points where the function has the same value. The atomic positions of a modulated crystal represent such a pattern, and the superspace group leaving the crystal invariant leads to a partition into equivalent atomic positions. These relations can be formulated either in $(3+d)$-dimensional space or, equally well, in three-dimensional space. As a simple case, we first consider a crystal with a one-dimensional occupation modulation: this implies $d=1$. Again, as in §9.8.1.3.2, we omit to indicate the basis vectors $\mathbf{d}_1$ and $\mathbf{d}_1^*$ and give only the corresponding components.

An element of the $(3+1)$-dimensional superspace group is a pair

$$g_s = (\{R|\mathbf{v}\}, \{\varepsilon|\upsilon_I\}) \qquad (9.8.4.36)$$

of Euclidean transformations in V and V_I, respectively. This element maps a point located at $r_s = (\mathbf{r}, t)$ to one at $(R\mathbf{r} + \mathbf{v}, \varepsilon t + \upsilon_I)$. Suppose the probability for the position $\mathbf{n} + \mathbf{r}_j$ to be occupied by an atom of species A is given by

$$P_A(\mathbf{n}, j, t) = p_j[\mathbf{q}\cdot(\mathbf{n} + \mathbf{r}_j) + t], \qquad (9.8.4.37)$$