International Tables for Crystallography (2006). Vol. A, Section 8.1.6, pp. 724–725.

We consider a crystal pattern with its vector lattice **L** referred to a primitive basis. Then, by definition, each vector of **L** has integral coefficients. The linear part of a symmetry operation maps **L** onto itself: $\mathbf{L} \rightarrow \boldsymbol{W}\mathbf{L} = \mathbf{L}$. Since the coefficients of all vectors of **L** are integers, the matrix $\boldsymbol{W}$ is an integral matrix, *i.e.* its coefficients are integers. Thus, the trace of $\boldsymbol{W}$, $\mathrm{tr}(\boldsymbol{W}) = W_{11} + \ldots + W_{nn}$, is also an integer. In $\mathbf{V}^3$, by reference to an appropriate orthonormal (not necessarily crystallographic) basis, one obtains another condition for the trace, $\mathrm{tr}(\boldsymbol{W}) = \pm(1 + 2\cos\varphi)$, where φ is the angle of rotation or rotoinversion. From these two conditions, it follows that φ can only be 0, 60, 90, 120, 180° *etc.*, and hence the familiar restriction to one-, two-, three-, four- and sixfold rotations and rotoinversions results.* These results imply for dimensions 2 and 3 that the matrix $\boldsymbol{W}$ satisfies the condition $(\boldsymbol{W})^k = \boldsymbol{I}$, with $k = 1, 2, 3, 4$ or 6.† Consequently, for the operation ($\boldsymbol{W}$, $\boldsymbol{w}$) in point space the relation

$$(\boldsymbol{W}, \boldsymbol{w})^k = [\boldsymbol{I}, (\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}] = (\boldsymbol{I}, \boldsymbol{t})$$

holds.

For the motion described by ($\boldsymbol{W}$, $\boldsymbol{w}$), this implies that a k-fold application results in a translation T (with translation vector **t**) of the crystal pattern. The (fractional) translation $(1/k)\mathsf{T}$ is called the *intrinsic translation part* (*screw or glide part*) of the symmetry operation. Whereas the 'translation part' of a motion depends on the choice of the origin, the 'intrinsic translation part' of a motion is uniquely determined. The intrinsic translation vector $(1/k)\mathbf{t}$ is the shortest translation vector of the motion for any choice of the origin.

If $\boldsymbol{t} = \boldsymbol{o}$, the symmetry operation has at least one fixed point and is a rotation, inversion, reflection or rotoinversion. If $\boldsymbol{t} \neq \boldsymbol{o}$, the term $(1/k)\mathbf{t}$ is called the *glide vector* (for a reflection) or the *screw vector* (for a rotation) of the symmetry operation. Both types of operations, glide reflections and screw rotations, have no fixed point.

For the geometric visualization of symmetry, the concept of *symmetry elements* is useful.‡ The symmetry element of a symmetry operation is the set of its fixed points, together with a characterization of the motion. For symmetry operations without fixed points (screw rotations or glide reflections), the fixed points of the corresponding rotations or reflections, described by $(\boldsymbol{W}, \boldsymbol{w}')$ with $\boldsymbol{w}' = \boldsymbol{w} - (1/k)\boldsymbol{t}$, are taken. Thus, in E^2, symmetry elements are N-fold rotation points (N = 2, 3, 4 or 6), mirror lines and glide lines. In E^3, symmetry elements are rotation axes, screw axes, inversion centres, mirror planes and glide planes. A peculiar situation exists for rotoinversions (except $\bar{1}$ and $\bar{2} \equiv m$). The symmetry element of such a rotoinversion consists of two components, a point and an axis. The point is the *inversion point* of the rotoinversion, and the *axis* of the rotoinversion is that of the corresponding rotation.

The determination of both the nature of a symmetry operation and the location of its symmetry element from the coordinate triplets, listed under *Positions* in the space-group tables, is described in Section 11.2.1 of Chapter 11.2.

8.1.6. Space groups and point groups

As mentioned in Section 8.1.3, the set of all symmetry operations of an object forms a group, the symmetry group of that object.

Definition: The symmetry group of a three-dimensional crystal pattern is called its *space group*. In E^2, the symmetry group of a (two-dimensional) crystal pattern is called its *plane group*. In E^1, the symmetry group of a (one-dimensional) crystal pattern is called its *line group*. To each crystal pattern belongs an infinite set of translations T_j which are symmetry operations of that pattern. The set of all T_j forms a group known as the *translation subgroup* $\mathcal{T}$ of the space group $\mathcal{G}$ of the crystal pattern. Since the commutative law $\mathsf{T}_j\mathsf{T}_k = \mathsf{T}_k\mathsf{T}_j$ holds for any two translations, $\mathcal{T}$ is an Abelian group.

With the aid of the translation subgroup $\mathcal{T}$, an insight into the architecture of the space group $\mathcal{G}$ can be gained.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, the space group $\mathcal{G}$ is described by the set $\{(\boldsymbol{W}, \boldsymbol{w})\}$ of matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. The group $\mathcal{T}$ is represented by the set of elements $(\boldsymbol{I}, \boldsymbol{t}_j)$, where $\boldsymbol{t}_j$ are the columns of coefficients of the translation vectors $\mathbf{t}_j$ of the lattice **L**. Let ($\boldsymbol{W}$, $\boldsymbol{w}$) describe an arbitrary symmetry operation W of $\mathcal{G}$. Then, all products $(\boldsymbol{I}, \boldsymbol{t}_j)(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)$ for the different j have the same matrix part $\boldsymbol{W}$. Conversely, every symmetry operation W of the space group with the same matrix part $\boldsymbol{W}$ is represented in the set $\{(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)\}$. The corresponding set of symmetry operations can be denoted by $\mathcal{T}\mathsf{W}$. Such a set is called a *right coset of* $\mathcal{G}$ *with respect to* $\mathcal{T}$, because the element W is the right factor in the products $\mathcal{T}\mathsf{W}$. Consequently, the space group $\mathcal{G}$ may be decomposed into the right cosets $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \mathcal{T}\mathsf{W}_3, \ldots, \mathcal{T}\mathsf{W}_i$, where the symmetry operations of the same column have the same matrix part $\boldsymbol{W}$, and the symmetry operations W_j differ by their matrix parts $\boldsymbol{W}_j$. This *coset decomposition of* $\mathcal{G}$ *with respect to* $\mathcal{T}$ may be displayed by the array

$$\begin{array}{lllll}
\mathsf{I} \equiv \mathsf{W}_1 & \mathsf{W}_2 & \mathsf{W}_3 & \ldots & \mathsf{W}_i \\
\mathsf{T}_1 & \mathsf{T}_1\mathsf{W}_2 & \mathsf{T}_1\mathsf{W}_3 & \ldots & \mathsf{T}_1\mathsf{W}_i \\
\mathsf{T}_2 & \mathsf{T}_2\mathsf{W}_2 & \mathsf{T}_2\mathsf{W}_3 & \ldots & \mathsf{T}_2\mathsf{W}_i \\
\mathsf{T}_3 & \mathsf{T}_3\mathsf{W}_2 & \mathsf{T}_3\mathsf{W}_3 & \ldots & \mathsf{T}_3\mathsf{W}_i \\
\vdots & \vdots & \vdots & & \vdots
\end{array}$$

Here, $\mathsf{W}_1 = \mathsf{I}$ is the identity operation and the elements of $\mathcal{T}$ form the first column, those of $\mathcal{T}\mathsf{W}_2$ the second column *etc.* As each column may be represented by the common matrix part $\boldsymbol{W}$ of its symmetry operations, the number i of columns, *i.e.* the number of cosets, is at the same time the number of *different* matrices $\boldsymbol{W}$ of the symmetry operations of $\mathcal{G}$. This number i is always finite, and is the order of the point group belonging to $\mathcal{G}$, as explained below. Any element of a coset $\mathcal{T}\mathsf{W}_j$ may be chosen as the representative element of that coset and listed at the top of its column. Choice of a different representative element merely results in a different order of the elements of a coset, but the coset does not change its content.§

Analogously, a coset $\mathsf{W}\mathcal{T}$ is called a *left coset* of $\mathcal{G}$ with respect to $\mathcal{T}$, and $\mathcal{G}$ can be decomposed into the left cosets $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \mathsf{W}_3\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. This left coset decomposition of a space group is always possible with the same $\mathsf{W}_1, \mathsf{W}_2, \ldots, \mathsf{W}_i$ as in the right coset decomposition. Moreover, both decompositions result in the same cosets, except for the order of the elements in each coset. A subgroup of a group with these properties is called a *normal subgroup* of the group; *cf.* Ledermann (1976). Thus, the translation subgroup $\mathcal{T}$ is a normal subgroup of the space group $\mathcal{G}$.

The decomposition of a space group into cosets is the basis of the description of the space groups in these *Tables*. The symmetry

* The reflection $m \equiv \bar{2}$ is contained among the rotoinversions. The same restriction is valid for the rotation angle φ in two-dimensional space, where $\mathrm{tr}(\boldsymbol{W}) = 2\cos\varphi$ if $\det(\boldsymbol{W}) = +1$. If $\det(\boldsymbol{W}) = -1$, $\mathrm{tr}(\boldsymbol{W}) = 0$ always holds and the operation is a reflection m.

† A method of deriving the possible orders of $\boldsymbol{W}$ in spaces of arbitrary dimension has been described by Hermann (1949).

‡ For a rigorous definition of the term *symmetry element*, see de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000).

§ A coset decomposition of a group $\mathcal{G}$ is possible with respect to every subgroup $\mathcal{H}$ of $\mathcal{G}$; *cf.* Ledermann (1976). The number of cosets is called the *index* [i] of $\mathcal{H}$ in $\mathcal{G}$. The integer [i] may be finite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to the (infinite) translation group $\mathcal{T}$ or infinite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to a (finite) site-symmetry group $\mathcal{S}$; *cf.* Section 8.3.2. If $\mathcal{G}$ is a finite group, a theorem of Lagrange states that the order of $\mathcal{G}$ is the product of the order of $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$.

operations of the space group are referred to a 'conventional' coordinate system (*cf.* Section 8.3.1) and described by $(n+1) \times (n+1)$ matrices. In the space-group tables as *general position* (*cf.* Section 8.3.2) for each column, a representative is listed whose coefficients w_j obey the condition $0 \leq w_j < 1$. The matrix is not listed completely, however, but is given in a short-hand notation. In the expression $W_{j1}x_1 + \ldots + W_{jn}x_n + w_j$, all vanishing terms and all $W_{jk} = 1$ are omitted, *e.g.*

$$\left.\begin{array}{l} 1x + 0y + 0z + \frac{1}{2} \\ 0x + 1y + 0z + 0 \\ 0x + 0y - 1z + \frac{1}{2} \end{array}\right\}$$

is replaced by $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$. The first entry of the general position is always the identity mapping, listed as x, y, z. It represents all translations of the space group too.

As groups, some space groups are more complicated than others. Most easy to survey are the 'symmorphic' space groups which may be defined as follows:

Definition: A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed.

In this case, the representative symmetry operations W_j of a symmorphic space group form a (finite) group. If the fixed point is chosen as the origin of the coordinate system, the column parts $\boldsymbol{w}_j$ of the representative symmetry operations W_j obey the equations $\boldsymbol{w}_j = \boldsymbol{o}$. Thus, for a symmorphic space group the representative symmetry operations may always be described by the special matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{o})$.

Symmorphic space groups may be easily identified by their Hermann–Mauguin symbols because these do not contain any glide or screw operation. For example, the monoclinic space groups with the symbols $P2$, $C2$, Pm, Cm, $P2/m$ and $C2/m$ are symmorphic, whereas those with the symbols $P2_1$, Pc, Cc, $P2_1/m, P2/c, P2_1/c$ and $C2/c$ are not.

Unlike most textbooks of crystallography, in this section point groups are treated after space groups because the space group of a crystal pattern, and thus of a crystal structure, determines its point group uniquely.

The external shape (morphology) of a macroscopic crystal is formed by its faces. In order to eliminate the influence of growth conditions, the set of crystal faces is replaced by the set of face normals, *i.e.* by a set of vectors. Thus, the symmetry group of the macroscopic crystal is the symmetry group of the *vector set of face normals.* It is not the group of motions in point space, therefore, that determines the symmetry of the macroscopic crystal, but the corresponding group of linear mappings of vector space; *cf.* Section 8.1.2. This group of linear mappings is called the *point group of the crystal.* Since to each macroscopic crystal a crystal structure corresponds and, furthermore, to each crystal structure a space group, the point group of the crystal defined above is also the point group of the crystal structure and the point group of its space group.

To connect more formally the concept of point groups with that of space groups in n-dimensional space, we consider the coset decomposition of a space group $\mathcal{G}$ with respect to the normal subgroup $\mathcal{T}$, as displayed above. We represent the right coset decomposition by $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \ldots, \mathcal{T}\mathsf{W}_i$ and the corresponding left coset decomposition by $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. If $\mathcal{G}$ is referred to a coordinate system, the symmetry operations of $\mathcal{G}$ are described by matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. As a result of the one-to-one correspondence between the i cosets $\mathcal{T}\mathsf{W}_j = \mathsf{W}_j\mathcal{T}$ and the i matrices $\boldsymbol{W}_j$, the cosets may alternatively be represented by the matrices $\boldsymbol{W}_j$. These matrices form a group of (finite) order i, and they describe linear mappings of the vector space $\mathbf{V}^n$ connected with E^n; *cf.* Section 8.1.2. This group (of order i) of linear mappings is the *point group $\mathcal{P}$ of the space group $\mathcal{G}$*, introduced above.

The difference between symmetry in point space and that in vector space may be exemplified again by means of some monoclinic space groups. Referred to conventional coordinate systems, space groups Pm, Pc, Cm and Cc have the same (3×3) matrices $\boldsymbol{W}_j$ of their symmetry operations. Thus, the point groups of all these space groups are of the same type m. The space groups themselves, however, show a rather different behaviour. In Pm and Cm reflections occur, whereas in Pc and Cc only glide reflections are present.

Remark: The usage of the term 'point group' in connection with space groups is rather unfortunate as the *point group of a space group* is *not* a group of motions of *point space* but a group acting on *vector space.* As a consequence, the point group of a space group may contain operations which do not occur in the space group at all. This is apparent from the example of monoclinic space groups above. Nevertheless, the term 'point group of a space group' is used here for historical reasons. A more adequate term would be 'vector point group' of a space group or a crystal. It must be mentioned that the term 'point group' is also used for the 'site-symmetry group', defined in Section 8.3.2. Site-symmetry groups are groups acting on point space.

It is of historic interest that the 32 types of three-dimensional crystallographic point groups were determined more than 50 years before the 230 (or 219) types of space group were known. The physical methods of the 19th century, *e.g.* the determination of the symmetry of the external shape or of tensor properties of a crystal, were essentially methods of determining the point group, not the space group of the crystal.

references