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Table 1.4.3.2
Generation of the space group $P6_122 \equiv D_6^2$ (178)

The entries in the second column designated by the numbers (1)–(12) correspond to the coordinate triplets of the general position of $P6_122$.

	Coordinate triplets	Symmetry operations
g_1	(1) x, y, z;	Identity I
g_2	$t(100)$	Generating translations
g_3	$t(010)$	
g_4	$t(001)$	
	The group $\mathcal{G}_4 \equiv \mathcal{T}$ of all translations of $P6_122$ has been generated	
g_5	(2) $\bar{y}, x-y, z+\frac{1}{3}$;	Threefold screw rotation
g_5^2	(3) $\bar{x}+y, \bar{x}, z+\frac{2}{3}$;	Threefold screw rotation
$g_5^3 = t(001)$:	Now the space group $\mathcal{G}_5 \equiv P3_1$ has been generated	
g_6	(4) $\bar{x}, \bar{y}, z+\frac{1}{2}$;	Twofold screw rotation
$g_6 * g_5$	(5) $y, \bar{x}+y, z+\frac{5}{6}$;	Sixfold screw rotation
$g_6 * g_5^2$	$x-y, x, z+\frac{7}{6} \sim$ (6) $x-y, x, z+\frac{1}{6}$;	Sixfold screw rotation
$g_6^2 = t(001)$:	Now the space group $\mathcal{G}_6 \equiv P6_1$ has been generated	
g_7	(7) $y, x, \bar{z}+\frac{1}{3}$;	Twofold rotation, direction of axis [110]
$g_7 * g_5$	(8) $x-y, \bar{y}, \bar{z}$;	Twofold rotation, axis [100]
$g_7 * g_5^2$	$\bar{x}, \bar{x}+y, \bar{z}-\frac{1}{3} \sim$ (9) $\bar{x}, \bar{x}+y, \bar{z}+\frac{2}{3}$;	Twofold rotation, axis [010]
$g_7 * g_6$	$\bar{y}, \bar{x}, \bar{z}-\frac{1}{6} \sim$ (10) $\bar{y}, \bar{x}, \bar{z}+\frac{5}{6}$;	Twofold rotation, axis [1$\bar{1}$0]
$g_7 * g_6 * g_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (11) $\bar{x}+y, y, \bar{z}+\frac{1}{2}$;	Twofold rotation, axis [120]
$g_7 * g_6 * g_5^2$	$x, x-y, \bar{z}-\frac{5}{6} \sim$ (12) $x, x-y, \bar{z}+\frac{1}{6}$;	Twofold rotation, axis [210]
$g_7^2 = I$	$\mathcal{G}_7 \sim P6_122$	

generators. Different choices of generators are possible. For the space-group tables, generators and generating procedures have been chosen such as to make the entries in the blocks 'General position' (*cf.* Section 2.1.3.11) and 'Symmetry operations' (*cf.* Section 2.1.3.9) as transparent as possible. Space groups of the same crystal class are generated in the same way (see Table 1.4.3.1 for the sequences that have been chosen), and the aim has been to accentuate important subgroups of space groups as much as possible. Accordingly, a process of generation in the form of a *composition series* has been adopted, see Ledermann (1976). The generator g_1 is defined as the identity operation, represented by (1) x, y, z. The generators g_2, g_3, and g_4 are the translations with translation vectors **a**, **b** and **c**, respectively. Thus, the coefficients k_2, k_3 and k_4 may have any integral value. If centring translations exist, they are generated by translations g_5 (and g_6 in the case of an F lattice) with translation vectors **d** (and **e**). For a C lattice, for example, **d** is given by $\mathbf{d} = \frac{1}{2}(\mathbf{a}+\mathbf{b})$. The exponents k_5 (and k_6) are restricted to the following values:

Lattice letter A, B, C, I: $k_5 = 0$ or 1.
Lattice letter R (hexagonal axes): $k_5 = 0$, 1 or 2.
Lattice letter F: $k_5 = 0$ or 1; $k_6 = 0$ or 1.

As a consequence, any translation t of $\mathcal{G}$ with translation vector

$$\mathbf{t} = k_2\mathbf{a} + k_3\mathbf{b} + k_4\mathbf{c}\,(+k_5\mathbf{d} + k_6\mathbf{e})$$

can be obtained as a product

$$t = (g_6)^{k_6}.(g_5)^{k_5}.g_4^{k_4}.g_3^{k_3}.g_2^{k_2}.g_1,$$

where $k_2, \ldots, k_6$ are integers determined by t. The generators g_6 and g_5 are enclosed between parentheses because they are effective only in centred lattices.

The remaining generators generate those symmetry operations that are not translations. They are chosen in such a way that only terms g_j or g_j^2 occur. For further specific rules, see below.

The process of generating the entries of the space-group tables may be demonstrated by the example in Table 1.4.3.2, where $\mathcal{G}_j$ denotes the group generated by $g_1, g_2, \ldots, g_j$. For $j \geq 5$, the next generator g_{j+1} is introduced when $g_j^{k_j} \in \mathcal{G}_{j-1}$, because in this case no new symmetry operation would be generated by $g_j^{k_j}$. The generating process is terminated when there is no further generator. In the present example, g_7 completes the generation: $\mathcal{G}_7 \equiv P6_122$ (178).

1.4.3.1. Selected order for non-translational generators

For the non-translational generators, the following sequence has been adopted:

(*a*) In all centrosymmetric space groups, an inversion (if possible at the origin O) has been selected as the last generator.

(*b*) Rotations precede symmetry operations of the second kind. In crystal classes $\bar{4}2m$ and $\bar{4}m2$ and $\bar{6}2m$ and $\bar{6}m2$, as an exception, $\bar{4}$ and $\bar{6}$ are generated first in order to take into account the conventional choice of origin in the fixed points of $\bar{4}$ and $\bar{6}$.

(*c*) The non-translational generators of space groups with C, A, B, F, I or R symbols are those of the corresponding space group with a P symbol, if possible. For instance, the generators of $I2_12_12_1$ (24) are those of $P2_12_12_1$ (19) and the generators of $Ibca$ (73) are those of $Pbca$ (61), apart from the centring translations.

Exceptions: $I4cm$ (108) and $I4/mcm$ (140) are generated *via* $P4cc$ (103) and $P4/mcc$ (124), because $P4cm$ and $P4/mcm$ do not exist. In space groups with d glides (except $I\bar{4}2d$, No. 122) and also in $I4_1/a$ (88), the corresponding rotation subgroup has been generated first. The generators of this subgroup are the same as those of the corresponding space group with a lattice symbol P.

Example
$F4_1/d\bar{3}2/m$ (227):
$P4_132$ (213) $\longrightarrow$ $F4_132$ (210) $\longrightarrow$ $F4_1/d\bar{3}2/m$.

(*d*) In some cases, rule (*c*) could not be followed without breaking rule (*a*), *e.g.* in *Cmme* (67). In such cases, the generators are chosen to correspond to the Hermann–Mauguin symbol as far as possible. For instance, the generators (apart from centring) of *Cmme* and *Imma* (74) are those of *Pmmb*, which is a non-standard setting of *Pmma* (51). (A combination of the generators of *Pmma* with the *C*- or *I*-centring translation results in non-standard settings of *Cmme* and *Imma*.)

For the space groups with lattice symbol *P*, the generation procedure has given the same triplets (except for their sequence) as in *IT* (1952). In non-*P* space groups, the triplets listed sometimes differ from those of *IT* (1952) by a centring translation.

1.4.4. General and special Wyckoff positions

By B. Souvignier

One of the first tasks in the analysis of crystal patterns is to determine the actual positions of the atoms. Since the full crystal pattern can be reconstructed from a single unit cell or even an asymmetric unit, it is clearly sufficient to focus on the atoms inside such a restricted volume. What one observes is that the atoms typically do not occupy arbitrary positions in the unit cell, but that they often lie on geometric elements, *e.g.* reflection planes or lines along rotation axes. It is therefore very useful to analyse the symmetry properties of the points in a unit cell in order to predict likely positions of atoms.

We note that in this chapter all statements and definitions refer to the usual three-dimensional space $\mathbb{E}^3$, but also can be formulated, *mutatis mutandis*, for plane groups acting on $\mathbb{E}^2$ and for higher-dimensional groups acting on n-dimensional space $\mathbb{E}^n$.

1.4.4.1. Crystallographic orbits

Since the operations of a space group provide symmetries of a crystal pattern, two points X and Y that are mapped onto each other by a space-group operation are regarded as being *geometrically equivalent*. Starting from a point $X \in \mathbb{E}^3$, infinitely many points Y equivalent to X are obtained by applying all space-group operations $g = (\boldsymbol{W}, \boldsymbol{w})$ to X: $Y = g(X) = (\boldsymbol{W}, \boldsymbol{w})X = (\boldsymbol{W}X + \boldsymbol{w})$.

Definition

For a space group $\mathcal{G}$ acting on the three-dimensional space $\mathbb{E}^3$, the (infinite) set

$$\mathcal{O} = \mathcal{G}(X) := \{g(X) | g \in \mathcal{G}\}$$

is called the *orbit of X under* $\mathcal{G}$.

The orbit of X is the smallest subset of $\mathbb{E}^3$ that contains X and is closed under the action of $\mathcal{G}$. It is also called a *crystallographic orbit*.

Every point in direct space $\mathbb{E}^3$ belongs to precisely one orbit under $\mathcal{G}$ and thus the orbits of $\mathcal{G}$ partition the direct space into disjoint subsets. It is clear that an orbit is completely determined by its points in the unit cell, since translating the unit cell by the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ entirely covers $\mathbb{E}^3$.

It may happen that two different symmetry operations g and h in $\mathcal{G}$ map X to the same point. Since $g(X) = h(X)$ implies that $h^{-1}g(X) = X$, the point X is fixed by the nontrivial operation $h^{-1}g$ in $\mathcal{G}$.

Definition

The subgroup $\mathcal{S}_X = \mathcal{S}_{\mathcal{G}}(X) := \{g \in \mathcal{G} | g(X) = X\}$ of symmetry operations from $\mathcal{G}$ that fix X is called the *site-symmetry group of X in* $\mathcal{G}$.

Since translations, glide reflections and screw rotations fix no point in $\mathbb{E}^3$, a site-symmetry group $\mathcal{S}_X$ never contains operations of these types and thus consists only of reflections, rotations, inversions and rotoinversions. Because of the absence of translations, $\mathcal{S}_X$ contains at most one operation from a coset $\mathcal{T}g$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$, since otherwise the quotient of two such operations tg and $t'g$ would be the nontrivial translation $tgg^{-1}t'^{-1} = tt'^{-1}$ (see Chapter 1.3 for a discussion of coset decompositions). In particular, the operations in $\mathcal{S}_X$ all have different linear parts and because these linear parts form a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$, the order of the site-symmetry group $\mathcal{S}_X$ is a divisor of the order of the point group of $\mathcal{G}$.

The site-symmetry group of a point X is thus a finite subgroup of the space group $\mathcal{G}$, a subgroup which is isomorphic to a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$.

Example

For a space group $\mathcal{G}$ of type $P\bar{1}$, the site-symmetry group of the origin $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ is clearly generated by the inversion in the origin: $\{\bar{1}|0\}(X) = X$. On the other hand, the point $Y = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ is fixed by the inversion in Y, *i.e.*

$$\{\bar{1}|1, 0, 1\}(Y) = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} = Y.$$

The symmetry operation $\{\bar{1}|1, 0, 1\}$ also belongs to $\mathcal{G}$ and generates the site-symmetry group of Y. The site-symmetry groups $\mathcal{S}_X = \{\{1|0\}, \{\bar{1}|0\}\}$ of X and $\mathcal{S}_Y = \{\{1|0\}, \{\bar{1}|1, 0, 1\}\}$ of Y are thus different subgroups of order 2 of $\mathcal{G}$ which are isomorphic to the point group of $\mathcal{G}$ (which is generated by $\bar{1}$).

The order $|\mathcal{S}_X|$ of the site-symmetry group $\mathcal{S}_X$ is closely related to the number of points in the orbit of X that lie in the unit cell. An application of the orbit–stabilizer theorem (see Section 1.1.7) yields the crucial observation that each point $Y = g(X)$ in the orbit of X under $\mathcal{G}$ is obtained precisely $|\mathcal{S}_X|$ times as an orbit point: for each $h \in \mathcal{S}_X$ one has $gh(X) = g(X) = Y$ and conversely $g'(X) = g(X)$ implies that $g^{-1}g' = h \in \mathcal{S}_X$ and thus $g' = gh$ for an operation h in $\mathcal{S}_X$.

Assuming first that we are dealing with a space group $\mathcal{G}$ described by a *primitive* lattice, each coset of $\mathcal{G}$ relative to the translation subgroup $\mathcal{T}$ contains precisely one operation g such that $g(X)$ lies in the primitive unit cell. Since the number of cosets equals the order $|\mathcal{P}|$ of the point group $\mathcal{P}$ of $\mathcal{G}$ and since each orbit point is obtained $|\mathcal{S}_X|$ times, it follows that the number of orbit points in the unit cell is $|\mathcal{P}|/|\mathcal{S}_X|$.

If we deal with a space group with a centred unit cell, the above result has to be modified slightly. If there are $k - 1$ centring vectors, the lattice spanned by the conventional basis is a sublattice of index k in the full translation lattice. The conventional cell therefore is built up from k primitive unit cells (spanned by a primitive lattice basis) and thus in particular contains k times as many points as the primitive cell (see Chapter 1.3 for a detailed discussion of conventional and primitive bases and cells).