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

  references