

8. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 8.3.5.2. Example of a space-group generation $\mathcal{G} : P6_122 \equiv D_6^2$ (No. 178)

	Coordinates	Symmetry operations
G_1	(1) x, y, z ;	Identity I
G_2	$t(100)$	$\left\{ \begin{array}{l} \text{These are the generating translations.} \\ \mathcal{G}_4 \text{ is the group } \mathcal{T} \text{ of all translations} \\ \text{of } P6_122 \end{array} \right.$
G_3	$t(010)$	
G_4	$t(001)$	
G_5	(2) $\bar{y}, x - y, z + \frac{1}{3}$;	
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 $[\bar{1}10]$
$G_7 * G_6 * G_5$	$\bar{x} + y, y, \bar{z} - \frac{1}{2} \sim$ (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]
$G_7^2 = I$	$\mathcal{G}_7 \sim P6_122$	

those of $Pmmb$, which is a non-standard setting of $Pmma$. (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.

8.3.6. Normalizers of space groups

The concept of normalizers, well known to mathematicians since the nineteenth century, is finding more and more applications in crystallography. Normalizers play an important role in the general theory of space groups of n -dimensional space. By the so-called Zassenhaus algorithm, one can determine the space-group types of n -dimensional space, provided the arithmetic crystal classes and for each arithmetic crystal class a representative integral $(n \times n)$ -matrix group are known. The crucial step is then to determine for these matrix groups their normalizers in $GL(n, Z)$. This was done for $n = 4$ by Brown *et al.* (1978) in the derivation of the 4894 space-group types. Now, the program package *Carat* solves this problem and was used, among others, for the enumeration of the 28 927 922 affine space-group types for six-dimensional space, see Table 8.1.1.1.

Crystallographers have been applying normalizers in their practical work for some time without realizing this fact, and only in the last decades have they become aware of the importance of normalizers. Normalizers first seem to have been derived visually, see Hirshfeld (1968). A derivation of the normalizers of the space groups using matrix methods is found in a paper by Boisen *et al.* (1990).

For the practical application of normalizers in crystallographic problems, see Part 15, which also contains detailed lists of normalizers of the point groups and space groups, as well as of space groups with special metrics. In this section, a short elementary introduction to normalizers will be presented.

In Section 8.1.6, the elements of a space group \mathcal{G} have been divided into classes with respect to the subgroup \mathcal{T} of all translations of \mathcal{G} ; these classes have been called *cosets*. ‘Coset decomposition’ can be performed for any pair ‘group \mathcal{G} and subgroup \mathcal{H} ’. The subgroup \mathcal{H} is called *normal* if the decomposition of \mathcal{G} into right and left cosets results in the same cosets.

The decomposition of the elements of a group \mathcal{G} into ‘conjugacy classes’ is equally important in crystallography. These classes are defined as follows:

Definition: The elements A and B of a group \mathcal{G} are said to be *conjugate in \mathcal{G}* , if there exists an element $G \in \mathcal{G}$ such that $B = G^{-1}AG$.

Example

The symmetry group $4mm$ of a square consists of the symmetry operations 1, 2, 4, 4^{-1} , m_x , m_y , m_d and $m_{d'}$, see Fig. 8.3.6.1. Vertex 1 is left invariant by 1 and $m_{d'}$, vertex 2 by 1 and m_d . The operations m_d and $m_{d'}$ are conjugate, because $m_{d'} = 4^{-1}m_d4$ holds, as are m_x and m_y ($m_y = 4^{-1}m_x4$), or 4 and 4^{-1} ($4^{-1} = m_x^{-1}4m_x$). The operations 1 and 2 have no conjugates.

As proved in mathematical textbooks, *e.g.* Ledermann (1976), conjugacy indeed subdivides a group into classes of elements. The unit element 1 always forms a conjugacy class for itself, as does any element that commutes with every other element of the group. For finite groups, the number of elements in a conjugacy class is a factor of the group order. In infinite groups, such as space groups, conjugacy classes may contain an infinite number of elements.

Conjugacy can be transferred from elements to groups. Let \mathcal{H} be a subgroup of \mathcal{G} . Then another subgroup \mathcal{H}' of \mathcal{G} is said to be *conjugate to \mathcal{H} in \mathcal{G}* , if there exists an element $G \in \mathcal{G}$, such that $\mathcal{H}' = G^{-1}\mathcal{H}G$. In this way, the set of all subgroups \mathcal{H}_i of a group \mathcal{G} is divided into *classes of conjugate subgroups* or *conjugacy classes of subgroups*. Conjugacy classes may contain different numbers of subgroups but, for finite groups, the number of subgroups in each class is always a factor of the order of the group. Conjugacy classes which contain only one subgroup are of special interest; they are called *normal subgroups*. There are always two trivial normal subgroups of a group \mathcal{G} : the group \mathcal{G} itself and the group \mathcal{I} consisting of the unit element 1 only. For space groups, the group \mathcal{T} of all translations of the group always forms a normal subgroup of \mathcal{G} .

In the above-mentioned example of the square, the subgroups $\{1, m_x\}$ and $\{1, m_y\}$ as well as $\{1, m_d\}$ and $\{1, m_{d'}\}$ each form conjugate pairs, whereas the subgroups $\{1, 2, 4, 4^{-1}\}$, $\{1, 2, m_x, m_y\}$, $\{1, 2, m_d, m_{d'}\}$ and $\{1, 2\}$ are normal subgroups.

The characterization of normal subgroups, \mathcal{H} must obey the condition $\mathcal{H} = G^{-1}\mathcal{H}G$ for all elements $G \in \mathcal{G}$, is identical with the one used in Section 8.1.6. This relation can also be expressed as