International Tables for Crystallography (2006). Vol. A, Section 8.3.6, pp. 738–739.

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	$t(100)$	These are the generating translations.
G_3	$t(010)$	$\mathcal{G}_4$ is the group $\mathcal{T}$ of all translations
G_4	$t(001)$	of $P6_122$
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 $[\bar{1}10]$
$G_7 * G_6 * G_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (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 4*mm* 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

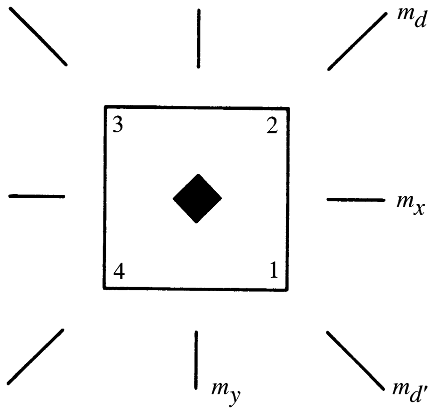

Fig. 8.3.6.1. Square with 'symmetry elements' m_x, m_y, m_d, $m_{d'}$ (mirror lines) and ◆ (fourfold rotation point). The vertices are numbered 1, 2, 3 and 4.

$\mathsf{G}\mathcal{H} = \mathcal{H}\mathsf{G}$ which means that the right and left cosets coincide. Thus each subgroup $\mathcal{H}$ of index [2] is normal, because there is only one coset in addition to $\mathcal{H}$ itself which is then necessarily the right as well as the left coset.

If $\mathcal{H}$ is not a normal subgroup of $\mathcal{G}$, then $\mathcal{H} = \mathsf{G}^{-1}\mathcal{H}\mathsf{G}$ cannot hold for all $\mathsf{G} \in \mathcal{G}$, because there is at least one subgroup $\mathcal{H}'$ of $\mathcal{G}$ which is conjugate to $\mathcal{H}$. This situation leads to the introduction of the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H}$ of $\mathcal{G}$.

Definition: The set of all elements $\mathsf{G} \in \mathcal{G}$, for which $\mathsf{G}^{-1}\mathcal{H}\mathsf{G} = \mathcal{H}$ holds, is called the *normalizer* $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of $\mathcal{H}$ in $\mathcal{G}$.

The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is always a group and thus a subgroup of $\mathcal{G}$ which obeys the relation $\mathcal{G} \geq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \trianglerighteq \mathcal{H}$. The symbol $\trianglerighteq$ means that $\mathcal{H}$ is a *normal* subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The subgroup $\mathcal{H}$ is normal in $\mathcal{G}$ if its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$ coincides with $\mathcal{G}$. Otherwise, other subgroups conjugate to $\mathcal{H}$ exist. To determine the number of conjugate subgroups of $\mathcal{H}$, one decomposes $\mathcal{G}$ into cosets relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The elements of each such coset transform $\mathcal{H}$ into a conjugate subgroup $\mathcal{H}'$, such that the number of conjugates (including $\mathcal{H}$ itself) equals the index of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in $\mathcal{G}$.

Examples

(1) The normalizer $\mathcal{N}_{4mm}(\{1, m_d\})$ of the subgroup $\{1, m_d\}$, see Fig. 8.3.6.1, consists of the elements $\{1, 2, m_d, m_{d'}\}$; its index in the full group $4mm$ of the square is [2]. Therefore, there are two conjugate subgroups $\{1, m_d\}$ and $\{1, m_{d'}\}$. All operations of the normalizer map the group $\{1, m_d\}$ onto itself and thus describe the 'symmetry in $4mm$ of this symmetry group'.

(2) Under space-group type $Fm\bar{3}m$ (No. 225), four subgroups of type $Pm\bar{3}m$ (No. 221) of index [4] are listed; four subgroups of type $Pn\bar{3}m$ (No. 224) are similarly listed. Are these subgroups conjugate in the original space group? Clearly, a space group of type $Pm\bar{3}m$ cannot be conjugate to one of the different type $Pn\bar{3}m$ because there exists no affine mapping transforming one into the other. On the other hand, one verifies that the four subgroups of type $Pm\bar{3}m$ are conjugate relative to $Fm\bar{3}m$: the transforming elements are the (centring) translations 000, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}0\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$. Similarly, the four subgroups of type $Pn\bar{3}m$ are conjugate in $Fm\bar{3}m$ by the same (centring) translations. The normalizers $\mathcal{N}_{Fm\bar{3}m}(Pm\bar{3}m)$ and $\mathcal{N}_{Fm\bar{3}m}(Pn\bar{3}m)$ are the subgroups themselves; their indices in $Fm\bar{3}m$ are [4], *i.e.* the numbers of conjugates are four.

Obviously, it would be impractical to list the normalizer for each type of group–subgroup pair. There are, however, some normalizers of outstanding importance from which, moreover, the normalizers determining the usual conjugacy relations can be obtained easily. Since space groups are groups of motions and space-group types are affine equivalence classes of space groups, *cf.* Sections 8.1.6 and 8.2.2, the groups $\mathcal{E}$ of *all* motions and $\mathcal{A}$ of *all* affine mappings are groups of special significance for any space group. The normalizers of a space group relative to these two groups are considered now. Part 15 contains lists of these normalizers with detailed comments.

The normalizer of a space group $\mathcal{G}$ in the group $\mathcal{A}$ of all affine mappings is called the *affine normalizer* $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of the space group $\mathcal{G}$. The affine normalizers of space groups of the same space-group type are affinely equivalent. One thus can speak of the 'type of normalizers of a space-group type'. In many cases, these normalizers are either space groups or isomorphic to space groups, but they may also be other groups due to arbitrarily small translations (for polar space groups) and/or due to noncrystallographic point groups (for triclinic and monoclinic space groups).

Affine normalizers are of more theoretical interest. For example, they determine the occurrence of enantiomorphism of space groups, *cf.* Section 8.2.2. A space-group type splits into a pair of enantiomorphic space-group types, if and only if its normalizers are contained in $\mathcal{A}^+$, the group of all affine mappings with positive determinant.

The normalizer of a space group $\mathcal{G}$ in the group $\mathcal{E}$ of all motions (Euclidean group) is called the *Euclidean normalizer* $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ of the space group $\mathcal{G}$. For all trigonal, tetragonal, hexagonal and cubic space groups, $\mathcal{N}_{\mathcal{E}} = \mathcal{N}_{\mathcal{A}}$ holds. In these cases, as well as in any context in which statements are valid for both normalizers, the abbreviated form $\mathcal{N}$ is frequently used.

The group $\mathcal{T}(\mathcal{N})$ of all translations of $\mathcal{N}$ is the same for both normalizers, $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, because any translation is a motion. It can be calculated easily: To be an element of $\mathcal{T}(\mathcal{N})$, the translation $(\boldsymbol{I}, \boldsymbol{t})$ has to satisfy the equation $(\boldsymbol{I}, \boldsymbol{t})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{t}) = (\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{G}$ for any operation $(\boldsymbol{W}, \boldsymbol{w})$ of $\mathcal{G}$. This results in $(\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}) = (\boldsymbol{W}', \boldsymbol{w}')$ or $\boldsymbol{W}' = \boldsymbol{W}$ and $\boldsymbol{w}' = \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}$. From this $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t} \in \mathcal{T}(\mathcal{G})$ follows, *i.e.* $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{t}$ must be a lattice translation of $\mathcal{G}$. To determine $\mathcal{T}(\mathcal{N})$, it is sufficient to apply this equation to the $\boldsymbol{W}_i$ of the generators of $\mathcal{G}$.

The conditions for the groups $\mathcal{T}(\mathcal{N})$ are the same for all space groups of the same arithmetic crystal class, because those space groups are generated by symmetry operations with the same matrix parts, and their lattices belong to the same centring type, if referred to conventional coordinate systems. The other elements of the normalizer are not obtained as easily.

In contrast to $\mathcal{N}_{\mathcal{A}}$, the type of $\mathcal{N}_{\mathcal{E}}$ is not a property of the space-group type, as the following example shows. The Euclidean normalizer of a space group $P222$ is an orthorhombic space group $Pmmm$ if $a \neq b \neq c \neq a$. It is a tetragonal space group if accidentally $a = b$ (or $b = c$ or $c = a$), and it is even cubic if accidentally $a = b = c$. The listings in Part 15 also contain the normalizers for the case of lattices with accidental symmetries.

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references