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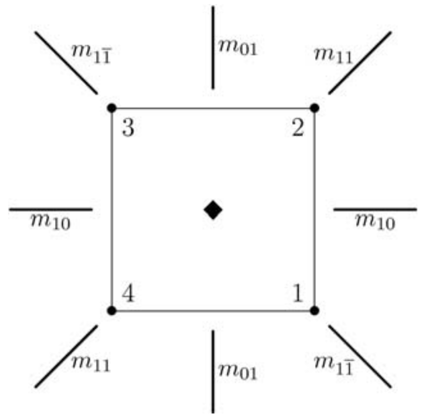

Figure 1.1.7.1
Stabilizers in the symmetry group $4mm$ of the square.

the *site-symmetry group* of P (in $\mathcal{G}$). These site-symmetry groups play a crucial role in the classification of positions in crystal structures. If the site-symmetry group of a point P consists only of the identity element of $\mathcal{G}$, P is called a point in *general position*, points with non-trivial site-symmetry groups are called points in *special position*.

According to the orbit–stabilizer theorem, points that are in the same orbit under the space group and which are thus symmetry equivalent have site-symmetry groups that are conjugate subgroups of $\mathcal{G}$. This gives rise to the concept of *Wyckoff positions*: points with site-symmetry groups that are conjugate subgroups of $\mathcal{G}$ belong to the same Wyckoff position. As a consequence, points in the same orbit under $\mathcal{G}$ certainly belong to the same Wyckoff position, but points may have the same site-symmetry group without being symmetry equivalent. The Wyckoff position of a point P consists of the union of the orbits of all points Q that have the same site-symmetry group as P. For a detailed discussion of the crucial notion of Wyckoff positions we refer to Section 1.4.4.

Example

In the symmetry group $4mm$ of the square the points $x, 0$ lying on the geometric element of m_{01} (*i.e.* the reflection line) are clearly stabilized by m_{01}. The origin $0, 0$ has the full group $4mm$ as its site-symmetry group, for all other points $x, 0$ with $x \neq 0$ the site-symmetry group is the group $\langle m_{01} \rangle$ generated by the reflection m_{01}.

The orbit of a point $P = x, 0$ with $x \neq 0$ is the four points $x, 0,\ \ 0, x,\ \ -x, 0,\ \ 0, -x$, where both $x, 0$ and $-x, 0$ have site-symmetry group $\langle m_{01} \rangle$ and $0, x$ and $0, -x$ have the conjugate site-symmetry group $\langle m_{10} \rangle$. This means that the Wyckoff position of *e.g.* the point $P = \frac{1}{2}, 0$ consists of the set of all points $x, 0$ and $0, x$ with arbitrary $x \neq 0$, *i.e.* of the union of the geometric elements of m_{01} and m_{10} with the exception of their intersection $0, 0$. A complete description of the distribution of points among the Wyckoff positions of the group $4mm$ is given in Table 3.2.3.1.

1.1.8. Conjugation, normalizers

In this section we focus on two group actions which are of particular importance for describing intrinsic properties of a group, namely the conjugation of group elements and the conjugation of subgroups. These actions were mentioned earlier in Section 1.1.5 when we introduced normal subgroups.

A group $\mathcal{G}$ acts on its elements *via* $g(h) := ghg^{-1}$, *i.e.* by conjugation. Note that the inverse element g^{-1} is required on the right-hand side of h in order to fulfil the rule $g(g'(h)) = (gg')(h)$ for a group action.

The orbits for this action are called the *conjugacy classes of elements* of $\mathcal{G}$ or simply *conjugacy classes* of $\mathcal{G}$; the conjugacy class of an element h consists of all its conjugates ghg^{-1} with g running over all elements of $\mathcal{G}$. Elements in one conjugacy class have *e.g.* the same order, and in the case of groups of symmetry operations they also share geometric properties such as being a reflection, rotation or rotoinversion. In particular, conjugate elements have the same type of geometric element.

The connection between conjugate symmetry operations and their geometric elements is even more explicit by the orbit–stabilizer theorem: If h and h' are conjugate by g, *i.e.* $h' = ghg^{-1}$, then g maps the geometric element of h to the geometric element of h'.

Example

The rotation group of a cube contains six fourfold rotations and if the cube is in standard orientation with the origin in its centre, the fourfold rotations 4^+_{100}, 4^+_{010} and 4^+_{001} and their inverses have the lines along the coordinate axes

$$\left\{ \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}, \left\{ \begin{pmatrix} 0 \\ y \\ 0 \end{pmatrix} \mid y \in \mathbb{R} \right\} \text{ and } \left\{ \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} \mid z \in \mathbb{R} \right\}$$

as their geometric elements, respectively. The twofold rotation 2_{110} around the line

$$\left\{ \begin{pmatrix} x \\ x \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}$$

maps the a axis to the b axis and *vice versa*, therefore the symmetry operation 2_{110} conjugates 4^+_{100} to a fourfold rotation with the line along the b axis as geometric element. Since the positive part of the a axis is mapped to the positive part of the b axis and conjugation also preserves the handedness of a rotation, 4^+_{100} is conjugated to 4^+_{010} and not to the inverse element 4^-_{010}. The line along the c axis is fixed by 2_{110}, but its orientation is reversed, *i.e.* the positive and negative parts of the c axis are interchanged. Therefore, 4^+_{001} is conjugated to its inverse 4^-_{001} by 2_{110}.

For the conjugation action, the stabilizer of an element h is called the *centralizer* $\mathcal{C}_{\mathcal{G}}(h)$ of h in $\mathcal{G}$, consisting of all elements in $\mathcal{G}$ that commute with h, *i.e.* $\mathcal{C}_{\mathcal{G}}(h) = \{g \in \mathcal{G} \mid gh = hg\}$.

Elements that form a conjugacy class on their own commute with all elements of $\mathcal{G}$ and thus have the full group as their centralizer. The collection of all these elements forms a normal subgroup of $\mathcal{G}$ which is called the *centre* of $\mathcal{G}$.

A group $\mathcal{G}$ acts on its subgroups *via* $g(\mathcal{H}) := g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$, *i.e.* by conjugating all elements of the subgroup. The orbits are called *conjugacy classes of subgroups* of $\mathcal{G}$. Considering the conjugation action of $\mathcal{G}$ on its subgroups is often convenient, because conjugate subgroups are in particular isomorphic: an isomorphism from $\mathcal{H}$ to $g\mathcal{H}g^{-1}$ is provided by the mapping $h \longmapsto ghg^{-1}$.

The stabilizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ under this conjugation action is called the *normalizer* $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of $\mathcal{H}$ in $\mathcal{G}$. The normalizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ is the largest subgroup $\mathcal{N}$ of $\mathcal{G}$ such that $\mathcal{H}$ is a normal subgroup of $\mathcal{N}$. In particular, a subgroup is a normal subgroup of $\mathcal{G}$ if and only if its normalizer is the full group $\mathcal{G}$.

The number of conjugate subgroups of $\mathcal{H}$ in $\mathcal{G}$ is equal to the index of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in $\mathcal{G}$. According to the orbit–stabilizer theorem, the different conjugate subgroups of $\mathcal{H}$ are obtained by conjugating $\mathcal{H}$ with coset representatives for the cosets of $\mathcal{G}$ relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$.

Examples

(i) In an abelian group $\mathcal{G}$, every element is only conjugate with itself, since $ghg^{-1} = h$ for all g, h in $\mathcal{G}$. Therefore each conjugacy class consists of just a single element.
Also, every subgroup $\mathcal{H}$ of an abelian group $\mathcal{G}$ is a normal subgroup, thus its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is $\mathcal{G}$ itself and $\mathcal{H}$ is only conjugate to itself.

(ii) The conjugacy classes of the symmetry group $3m$ of an equilateral triangle are $\{1\}$, $\{m_{10}, m_{01}, m_{11}\}$ and $\{3^+, 3^-\}$. The centralizer of m_{10} is just the group $\langle m_{10}\rangle$ generated by m_{10}, *i.e.* 1 and m_{10} are the only elements of $3m$ commuting with m_{10}. Analogously, one sees that the centralizer $\mathcal{C}_{\mathcal{G}}(h) = \langle h\rangle$ for each element h in $3m$, except for $h = 1$.
The subgroups $\langle m_{10}\rangle$, $\langle m_{01}\rangle$ and $\langle m_{11}\rangle$ are conjugate subgroups (with conjugating elements 3^+ and 3^-). These subgroups coincide with their normalizers, since they have index 3 in the full group.

(iii) The conjugacy classes of the symmetry group $4mm$ of a square are $\{1\}$, $\{2\}$, $\{m_{10}, m_{01}\}$, $\{m_{11}, m_{1\bar{1}}\}$ and $\{4^+, 4^-\}$. Since 2 forms a conjugacy class on its own, this is an element in the centre of $4mm$ and its centralizer is the full group. The centralizer of m_{10} is $\langle m_{10}, m_{01}\rangle$, which is also the centralizer of m_{01} (note that m_{10} and m_{01} are reflections with normal vectors perpendicular to each other, and thus commute). Analogously, $\langle m_{11}, m_{1\bar{1}}\rangle$ is the centralizer of both m_{11} and $m_{1\bar{1}}$. Finally, 4^+ only commutes with the rotations in $4mm$, therefore its centralizer is $\langle 4^+\rangle$.
The five subgroups of order 2 in $4mm$ fall into three conjugacy classes, namely the normal subgroup $\langle 2\rangle$ and the two pairs $\{\langle m_{10}\rangle, \langle m_{01}\rangle\}$ and $\{\langle m_{11}\rangle, \langle m_{1\bar{1}}\rangle\}$. The normalizer of both $\langle m_{10}\rangle$ and $\langle m_{01}\rangle$ is $\langle 2, m_{10}\rangle$ and the normalizer of both $\langle m_{11}\rangle$ and $\langle m_{1\bar{1}}\rangle$ is $\langle 2, m_{11}\rangle$.

In the context of crystallographic groups, conjugate subgroups are not only isomorphic, but have the same types of geometric elements, possibly with different directions. In many situations it is therefore sufficient to restrict attention to representatives of the conjugacy classes of subgroups. Furthermore, conjugation with elements from the normalizer of a group $\mathcal{H}$ permutes the geometric elements of the symmetry operations of $\mathcal{H}$. The role of the normalizer may in this situation be expressed by the phrase

The normalizer describes the *symmetry of the symmetries*.

Thus, the normalizer reflects an intrinsic ambiguity between different but equivalent descriptions of an object by its symmetries.

Example

The subgroup $\mathcal{H} = \langle 2, m_{10}\rangle$ is a normal subgroup of the symmetry group $\mathcal{G} = 4mm$ of the square, and thus $\mathcal{G}$ is the normalizer of $\mathcal{H}$ in $\mathcal{G}$. As can be seen in the diagram in Fig. 1.1.7.1, the fourfold rotation 4^+ maps the geometric element of the reflection m_{10} to the geometric element of m_{01} and *vice versa*, and fixes the geometric element of the rotation 4^+. Consequently, conjugation by 4^+ fixes $\mathcal{H}$ as a set, but interchanges the reflections m_{10} and m_{01}. These two reflections are geometrically indistinguishable, since their geometric elements are both lines through the centres of opposite edges of the square.
Analogously, 4^+ interchanges the geometric elements of the reflections m_{11} and $m_{1\bar{1}}$ of the subgroup $\mathcal{H}' = \langle 2, m_{11}\rangle$. These are the two reflection lines through opposite corners of the square.
In contrast to that, $\mathcal{G}$ does not contain an element mapping the geometric element of m_{10} to that of m_{11}. Note that an eightfold rotation would be such an element, but this is, however, not a symmetry of the square. The reflections m_{10} and m_{11} are thus geometrically different symmetry operations of the square.

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