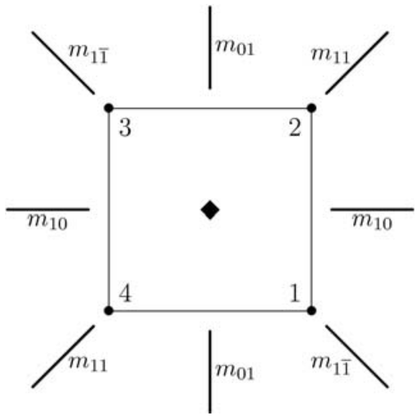


**Figure 1.1.7.1**
Stabilizers in the symmetry group $4mm$ of the square.

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 $\mathcal{G}$.