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position coordinates, normalizing to values between 0 and 1 (by adding ±1 if required) and eliminating duplicates.

For example, for the point $X = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$ in Wyckoff position 2*b* one obtains X and $Y = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}$ as the points in the orbit of X that lie in the unit cell. Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_X$ is a group of order 8/2 = 4. Its four operations are

Coordinate triplet	Description
x, y, z	Identity operation
$\bar{x}+1, \bar{y}, z$	Twofold rotation with axis $\frac{1}{2}, 0, z$
$\bar{y}+\frac{1}{2}, \bar{x}+\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, -x, z$
$y+\frac{1}{2}, x-\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, x, z$

The corresponding oriented symbol for the site-symmetry is 2.*mm*, indicating that the site-symmetry group contains a twofold rotation along a primary lattice direction, no symmetry operations along the secondary directions and two reflections along tertiary directions.

Since X and Y lie in the same orbit, they clearly belong to the same Wyckoff position. But every point $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$ has the same site-symmetry group as X and therefore also belongs to the same Wyckoff position as X. Inserting the coordinates of X' in the general-position coordinates, one obtains $Y' = \begin{pmatrix} 0 \\ \frac{1}{2} \\ z \end{pmatrix}$ as the only other point in the orbit of X' that lies in the unit cell. Clearly, Y' has the same site-symmetry group as Y. The Wyckoff position 2*b* to which X belongs therefore consists of the union of the orbits of the points $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$.

In the space-group diagram in Fig. 1.4.4.2, the points belonging to Wyckoff position 2*b* can be identified as the points on the intersection of a twofold rotation axis directed along [001] and two reflection planes normal to the square diagonals and crossing the centres of the sides bordering the unit cell. It is clear that for every value of z, the four intersection points in the unit cell lie in one orbit under the fourfold rotation located in the centre of the displayed cell.

Applying the same procedure to a point $X = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$ in Wyckoff position 2*a*, the points in the orbit that lie in the unit cell are seen to be X and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ z \end{pmatrix}$. The site-symmetry group $\mathcal{S}_X$ is again of order 4 and since the fourfold rotation $\{4^+|0\}$ fixes X, $\mathcal{S}_X$ is the cyclic group of order 4 generated by this fourfold rotation. The oriented symbol for this site-symmetry group is 4.. and the corresponding points can easily be identified in the space-group diagram in Fig. 1.4.4.2 by the symbol for a fourfold rotation.

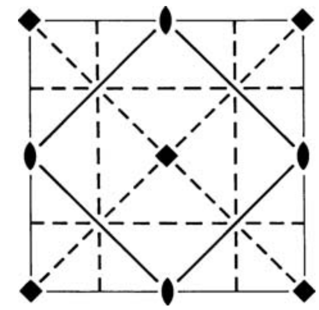

Figure 1.4.4.2
Symmetry-element diagram for the space group *P*4*bm* (100) for the orthogonal projection along [001].

Since a point in a special position has to lie on the geometric element of a reflection, rotation or inversion, the special positions can in principle be read off from the space-group diagrams. In the present example, we have dealt with the positions fixed by twofold or fourfold rotations, and from the diagram in Fig. 1.4.4.2 one sees that the only remaining case is that of points on reflection planes, indicated by the solid lines. A point on such a reflection plane is $X = \begin{pmatrix} x \\ x+\frac{1}{2} \\ z \end{pmatrix}$ and by inserting these coordinates into the general-position coordinates one obtains the points $\bar{x}, \bar{x}+\frac{1}{2}, z$, $\bar{x}+\frac{1}{2}, x, z$ and $x+\frac{1}{2}, \bar{x}, z$ as the other points in the orbit of X (up to translations). Here, the site-symmetry group $\mathcal{S}_X$ is of order 2, it is generated by the reflection $\{m_{1\bar{1}0}| -\frac{1}{2}, \frac{1}{2}, 0\}$: $y-\frac{1}{2}, x+\frac{1}{2}, z$ having the plane $x, x+\frac{1}{2}, z$ as geometric element. The oriented symbol of $\mathcal{S}_X$ is ..*m*, since the reflection is along a tertiary direction.

1.4.4.3. Wyckoff sets

Points belonging to the same Wyckoff position have conjugate site-symmetry groups and thus in particular all those points are collected together that lie in one orbit under the space group $\mathcal{G}$. However, in addition, points that are not symmetry-related by a symmetry operation in $\mathcal{G}$ may still play geometrically equivalent roles, *e.g.* as intersections of rotation axes with certain reflection planes.

Example

In the conventional setting, the fourfold axes of a space group $\mathcal{G}$ of type *P*4 (75) intersect the *ab* plane in the points $u_1, u_2, 0$ and $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ for integers u_1, u_2, as can be seen from the space-group diagram in Fig. 1.4.4.3.

The points $u_1, u_2, 0$ lie in one orbit under the translation subgroup of $\mathcal{G}$, and thus belong to the same Wyckoff position, labelled 1*a*. For the same reason, the points $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ belong to a single Wyckoff position, namely to position 1*b*. The points $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ do not belong to the same Wyckoff position, because the site-symmetry group $\mathcal{S}_X$ is generated by the fourfold rotation 4_{001} and conjugating this by an operation $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$ results in a fourfold rotation with axis parallel to the *c* axis and running through $\boldsymbol{w}$. But since the translation parts of all operations in $\mathcal{G}$ are integral, such an axis

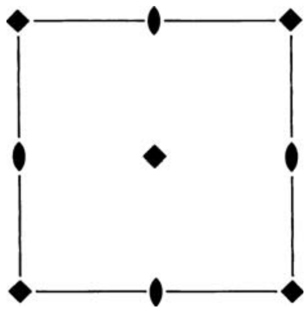

Figure 1.4.4.3
Symmetry-element diagram for the space group $P4$ (75) for the orthogonal projection along [001].

can not contain $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and thus $\mathcal{S}_X$ and $\mathcal{S}_Y$ are not conjugate in $\mathcal{G}$.
However, the translation by $(\frac{1}{2}, \frac{1}{2}, 0)$ conjugates $\mathcal{S}_X$ to $\mathcal{S}_Y$, while fixing the group $\mathcal{G}$ as a whole. This shows that there is an ambiguity in choosing the origin either at $0, 0, 0$ or $\frac{1}{2}, \frac{1}{2}, 0$, since these points are geometrically indistinguishable (both being intersections of a fourfold axis with the *ab* plane).

The ambiguity in the origin choice in the above example can be explained by the *affine normalizer* of the space group $\mathcal{G}$ (see Section 1.1.8 for a general introduction to normalizers). The full group $\mathcal{A}$ of affine mappings acts *via* conjugation on the set of space groups and the space groups of the same affine type are obtained as the orbit of a single group of that type under $\mathcal{A}$.

Definition
The group $\mathcal{N}$ of affine mappings $n \in \mathcal{A}$ that fix a space group $\mathcal{G}$ under conjugation is called the *affine normalizer* of $\mathcal{G}$, *i.e.*

$$\mathcal{N} = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = \{n \in \mathcal{A} | n\mathcal{G}n^{-1} = \mathcal{G}\}.$$

The affine normalizer is the largest subgroup of $\mathcal{A}$ such that $\mathcal{G}$ is a normal subgroup of $\mathcal{N}$.

Conjugation by operations of the affine normalizer results in a permutation of the operations of $\mathcal{G}$, *i.e.* in a relabelling without changing their geometric properties. The additional translations contained in the affine normalizer can in fact be derived from the space-group diagrams, because shifting the origin by such a translation results in precisely the same diagram. More generally, an element of the affine normalizer can be interpreted as a change of the coordinate system that does not alter the space-group diagrams.

A more thorough description of the affine normalizers of space groups is given in Chapter 3.5, where tables with the affine normalizers are also provided.

Since the affine normalizer of a space group $\mathcal{G}$ is in general a group containing $\mathcal{G}$ as a proper subgroup, it is possible that subgroups of $\mathcal{G}$ that are not conjugate by any operation of $\mathcal{G}$ may be conjugate by an operation in the affine normalizer. As a consequence, the site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ of two points X and Y belonging to different Wyckoff positions of $\mathcal{G}$ may be conjugate under the affine normalizer of $\mathcal{G}$. This reveals that the points X and Y are in fact geometrically equivalent, since they fall into the same orbit under the affine normalizer of $\mathcal{G}$. Joining the equivalence classes of these points into a single class results in a coarser classification with larger classes, which are called *Wyckoff sets*.

Definition
Two points X and Y belong to the same *Wyckoff set* if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of the affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$.
In particular, the Wyckoff set containing a point X also contains the full orbit of X under the affine normalizer of $\mathcal{G}$.

Example
Let $\mathcal{G}$ be the space group of type $P222_1$ (17) generated by the translations of an orthorhombic lattice, the twofold rotation $\{2_{100}|0\}$: $x, \bar{y}, \bar{z}$ and the twofold screw rotation $\{2_{001}|0, 0, \frac{1}{2}\}$: $\bar{x}, \bar{y}, z + \frac{1}{2}$. Note that the composition of these two elements is the twofold rotation with the line $0, y, \frac{1}{4}$ as its geometric element. The group $\mathcal{G}$ has four different Wyckoff positions with a site-symmetry group generated by a twofold rotation; representatives of these Wyckoff positions are the points $X_1 = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ (Wyckoff position 2*a*, site-symmetry symbol 2..), $X_2 = \begin{pmatrix} x \\ \frac{1}{2} \\ 0 \end{pmatrix}$ (position 2*b*, symbol 2..), $Y_1 = \begin{pmatrix} 0 \\ y \\ \frac{1}{4} \end{pmatrix}$ (position 2*c*, symbol .2.) and $Y_2 = \begin{pmatrix} \frac{1}{2} \\ y \\ \frac{1}{4} \end{pmatrix}$ (position 2*d*, symbol .2.).
From the tables of affine normalizers in Chapter 3.5, but also by a careful analysis of the space-group diagrams in Fig. 1.4.4.4, one deduces that the affine normalizer of $\mathcal{G}$ contains the additional translations $t(\frac{1}{2}, 0, 0)$, $t(0, \frac{1}{2}, 0)$ and $t(0, 0, \frac{1}{2})$, since all the diagrams are invariant by a shift of $\frac{1}{2}$ along any of the coordinate axes. Moreover, the symmetry operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$: $y, x, z + \frac{1}{4}$ which interchanges the a and b axes and shifts the origin by $\frac{1}{4}$ along the c axis belongs to the affine

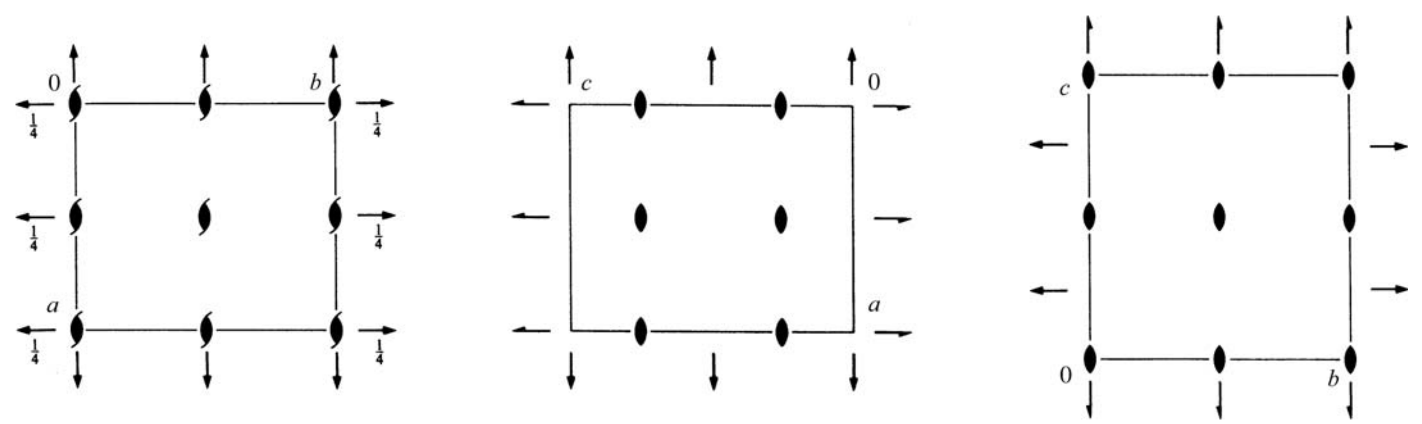

Figure 1.4.4.4
Symmetry-element diagrams for the space group $P222_1$ (17) for orthogonal projections along [001], [010], [100] (left to right).

normalizer, because it precisely interchanges the twofold rotations around axes parallel to the *a* and to the *b* axes. The translation $t(0, \frac{1}{2}, 0)$ maps X_1 to X_2, and hence X_1 and X_2 have site-symmetry groups which are conjugate under the affine normalizer of $\mathcal{G}$ and thus belong to the same Wyckoff set. Analogously, Y_1 and Y_2 belong to the same Wyckoff set, because $t(\frac{1}{2}, 0, 0)$ maps Y_1 to Y_2. Finally, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ found in the affine normalizer maps X_1 to Y_1. This shows that the points of all four Wyckoff positions actually belong to the same Wyckoff set.

Geometrically, the positions in this Wyckoff set can be described as those points that lie on a twofold rotation axis.

The assignments of Wyckoff positions of plane and space groups to Wyckoff sets are discussed and tabulated in Chapter 3.4.

Remark: The previous example deserves some further discussion. The group $\mathcal{G}$ of type $P222_1$ belongs to the orthorhombic crystal family, and the conventional unit cell is spanned by three basis vectors **a**, **b**, **c** with lengths a, b, c and right angles between each pair of basis vectors. Unless the parameters a and b are equal because of some metric specialization, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ of the affine normalizer is not an isometry but changes lengths. If it is desired that the metric properties are preserved, the full affine normalizer cannot be taken into account, but only the subgroup that consists of isometries. This subgroup is called the *Euclidean normalizer* of $\mathcal{G}$. (A detailed discussion of Euclidean normalizers of space groups and their tabulation are given in Chapter 3.5.)

Taking conjugacy of the site-symmetry groups under the Euclidean normalizer as a condition results in a notion of equivalence which lies between that of Wyckoff positions and Wyckoff sets. In the above example, the four Wyckoff positions would be merged into two classes represented by X_1 and Y_1, but X_1 and Y_1 would not be regarded as equivalent, since they are not related by an operation of the Euclidean normalizer.

It turns out, however, that in many cases this intermediate classification coincides with the Wyckoff sets, because points belonging to different Wyckoff positions are often related to each other by a translation contained in the affine normalizer. Since translations are always isometries, the translations contained in the affine normalizer always belong to the Euclidean normalizer as well.

1.4.4.4. Eigensymmetry groups and non-characteristic orbits

A crystallographic orbit $\mathcal{O}$ has been defined as the set of points $g(X)$ obtained by applying all operations of some space group $\mathcal{G}$ to a point $X \in \mathbb{E}^3$. From that it is clear that the set $\mathcal{O}$ is invariant as a whole under the action of operations in $\mathcal{G}$, since for some point $Y = g(X)$ in the orbit and $h \in \mathcal{G}$ one has $h(Y) = (hg)(X)$, which is again contained in $\mathcal{O}$ because hg belongs to $\mathcal{G}$. However, it is possible that the orbit $\mathcal{O}$ is also invariant under some isometries of $\mathbb{E}^3$ that are not contained in $\mathcal{G}$. Since the composition of two such isometries still keeps the orbit invariant, the set of all isometries leaving $\mathcal{O}$ invariant forms a group which contains $\mathcal{G}$ as a subgroup.

Definition

Let $\mathcal{O} = \{g(X) | g \in \mathcal{G}\}$ be the orbit of a point $X \in \mathbb{E}^3$ under a space group $\mathcal{G}$. Then the group $\mathcal{E}$ of isometries of $\mathbb{E}^3$ which leave $\mathcal{O}$ invariant as a whole is called the *eigensymmetry group* of $\mathcal{O}$.

Since the orbit is a discrete set, the eigensymmetry group has to be a space group itself. One distinguishes the following cases:

(i) The eigensymmetry group $\mathcal{E}$ equals the group $\mathcal{G}$ by which the orbit was generated. In this case the orbit is called a *characteristic orbit* of $\mathcal{G}$.

(ii) The eigensymmetry group $\mathcal{E}$ contains $\mathcal{G}$ as a proper subgroup. Then the orbit is called a *non-characteristic orbit*.

(iii) If the eigensymmetry group $\mathcal{E}$ contains translations that are not contained in $\mathcal{G}$, *i.e.* if $\mathcal{T}_{\mathcal{G}}$ is a proper subgroup of $\mathcal{T}_{\mathcal{E}}$, the orbit is called an *extraordinary orbit*. Of course, extraordinary orbits are a special kind of non-characteristic orbits.

Non-characteristic orbits are closely related to the concept of *lattice complexes*, which are discussed in Chapter 3.4. An extensive listing of non-characteristic orbits of space groups can be found in Engel *et al.* (1984).

The fact that an orbit of a space group has a larger eigensymmetry group is an important example of a pair of groups that are in a group–subgroup relation. Knowledge of subgroups and supergroups of a given space group play a crucial role in the analysis of phase transitions, for example, and are discussed in detail in Chapter 1.7.

The occurrence of non-characteristic orbits does not require the point X to be chosen at a special position. Even the general position of a space group $\mathcal{G}$ may give rise to a non-characteristic orbit. Moreover, special values of the coordinates of the general position may give rise to additional eigensymmetries without the position becoming a special position. Conversely, the orbit of a point at a special position need not be non-characteristic.

Example

We compare space groups of types $P4_1$ (76) and $P4_2$ (77). For a space group of type $P4_1$, the general position with generic coordinates x, y, z gives rise to a characteristic orbit, whereas the general-position orbit for a space group of type $P4_2$ consists of the points $X_1 = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, $X_2 = \begin{pmatrix} \bar{x} \\ \bar{y} \\ z \end{pmatrix}$, $X_3 = \begin{pmatrix} \bar{y} \\ x \\ z + \frac{1}{2} \end{pmatrix}$ and $X_4 = \begin{pmatrix} y \\ \bar{x} \\ z + \frac{1}{2} \end{pmatrix}$. An inversion $\{\bar{1}|0, 0, 2z\}$ in $0, 0, z$ interchanges X_1 and X_2, and maps X_3 to $y, \bar{x}, z - \frac{1}{2}$, which is clearly equivalent to X_4 under a translation. This shows that the general-position orbit for a space group of type $P4_2$ is a non-characteristic orbit, and the eigensymmetry group of this orbit is of type $P4_2/m$ (84), where the origin has to be shifted to the inversion point $0, 0, z$ to obtain the conventional setting. Since the unit cell and the orbit are unchanged, but the point group of $P4_2$ is a subgroup of index 2 in the point group of $P4_2/m$, the orbit points must belong to a special position for $P4_2/m$, namely the position labelled $4j$. In the conventional setting of $P4_2/m$, a point belonging to this Wyckoff position is given by x, y, 0 and one finds that the orbit of this point in special position is characteristic, *i.e.* its eigensymmetry group is just $P4_2/m$.

If we assume that the metric of the space group is not special, the eigensymmetry group is restricted to the same crystal family (for the definition of 'specialized' metrics, *cf.* Section 1.3.4.3 and Chapter 3.5). Therefore, a space group $\mathcal{G}$ for which the point group is a holohedry can only have non-characteristic orbits by additional translations, *i.e.* extraordinary orbits. However, if we allow specialized metrics, the eigensymmetry group may belong to a higher crystal family. For example, if a space group belongs to the orthorhombic family, but the unit cell has equal parameters