International Tables for Crystallography (2016). Vol. A, Figure 1.4.4.2, p. 64.

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 $2b$ 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 $2b$ 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 $2b$ 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 $2a$, 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.

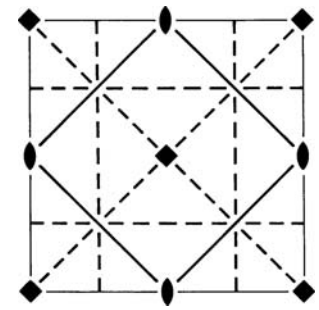

Figure 1.4.4.2
Symmetry-element diagram for the space group $P4bm$ (100) for the orthogonal projection along [001].

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 $P4$ (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 $1a$. 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 $1b$. 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

references