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Proposition

Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and let $\mathcal{S}_X$ be the site-symmetry group of a point X in $\mathbb{E}^3$. Then the number of orbit points of the orbit of X which lie in a conventional cell for $\mathcal{G}$ is equal to the product $k \times |\mathcal{P}|/|\mathcal{S}_X|$, where k is the volume of the conventional cell divided by the volume of a primitive unit cell.

1.4.4.2. Wyckoff positions

As already mentioned, one of the first issues in the analysis of crystal structures is the determination of the actual atom positions. Energetically favourable configurations in inorganic compounds are often achieved when the atoms occupy positions that have a nontrivial site-symmetry group. This suggests that one should classify the points in $\mathbb{E}^3$ into equivalence classes according to their site-symmetry groups.

Definition

A point $X \in \mathbb{E}^3$ is called a point in a *general position* for the space group $\mathcal{G}$ if its site-symmetry group contains only the identity element of $\mathcal{G}$. Otherwise, X is called a point in a *special position*.

The distinctive feature of a point in a general position is that the points in its orbit are in one-to-one correspondence with the symmetry operations of the group $\mathcal{G}$ by associating the orbit point $g(X)$ with the group operation g. For different group elements g and g', the orbit points $g(X)$ and $g'(X)$ must be different, since otherwise $g^{-1}g'$ would be a non-trivial operation in the site-symmetry group of X. Therefore, the entries listed in the space-group tables for the general positions can not only be interpreted as a shorthand notation for the symmetry operations in $\mathcal{G}$ (as seen in Section 1.4.2.3), but also as coordinates of the points in the orbit of a point X in a general position with coordinates x, y, z (up to translations).

Whereas points in general positions exist for every space group, not every space group has points in a special position. Such groups are called *fixed-point-free space groups* or *Bieberbach groups* and are precisely those groups that may contain glide reflections or screw rotations, but no proper reflections, rotations, inversions and rotoinversions.

Example

The group $\mathcal{G}$ of type $Pna2_1$ (33) has a point group of order 4 and representatives for the non-trivial cosets relative to the translation subgroup are the twofold screw rotation $\bar{x}, \bar{y}, z+\frac{1}{2}$, the a glide $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$ and the n glide $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$. No operation in the coset of the twofold screw rotation can have a fixed point, since such an operation maps the z component to $z+\frac{1}{2}+t_z$ for an integer t_z, and this is never equal to z. The same argument applies to the x component of the a glide and to the y component of the n glide, hence this group contains no operation with a fixed point (apart from the identity element) and is thus a fixed-point-free space group.

The distinction into general and special positions is of course very coarse. In a finer classification, it is certainly desirable that two points in the same orbit under the space group belong to the same class, since they are symmetry equivalent. Such points have *conjugate* site-symmetry groups (*cf.* the orbit–stabilizer theorem in Section 1.1.7).

Lemma

Let X and Y be points in the same orbit of a space group $\mathcal{G}$ and let $g \in \mathcal{G}$ such that $g(X) = Y$. Then the site-symmetry groups of X and Y are conjugate by the operation mapping X to Y, *i.e.* one has $\mathcal{S}_Y = g \cdot \mathcal{S}_X \cdot g^{-1}$.

The classification motivated by the conjugacy relation between the site-symmetry groups of points in the same orbit is the classification into *Wyckoff positions*.

Definition

Two points X and Y in $\mathbb{E}^3$ belong to the same *Wyckoff position* with respect to $\mathcal{G}$ if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of $\mathcal{G}$.

In particular, the Wyckoff position containing a point X also contains the full orbit $\mathcal{G}(X)$ of X under $\mathcal{G}$.

Remark: It is built into the definition of Wyckoff positions that points that are related by a symmetry operation of $\mathcal{G}$ belong to the same Wyckoff position. However, a single site-symmetry group may have more than one fixed point, *e.g.* points on the same rotation axis or in the same reflection plane. These points are in general not symmetry related but, having identical site-symmetry groups, clearly belong to the same Wyckoff position. This situation can be analyzed more explicitly:

Let $\mathcal{S}_X$ be the site-symmetry group of the point X and assume that Y is another point with the same site-symmetry group $\mathcal{S}_Y = \mathcal{S}_X$. Choosing a coordinate system with origin X, the operations in $\mathcal{S}_X$ all have translational part equal to zero and are thus matrix–column pairs of the form $(\boldsymbol{W}, \boldsymbol{o})$. In particular, these operations are *linear* operations, and since both points X and Y are fixed by all operations in $\mathcal{S}_X$, the vector $\mathbf{v} = Y - X$ is also fixed by the linear operations $(\boldsymbol{W}, \boldsymbol{o})$ in $\mathcal{S}_X$. But with the vector $\mathbf{v}$ each scaling $c \cdot \mathbf{v}$ of $\mathbf{v}$ is fixed as well, and therefore all the points on the line through X and Y are fixed by the operations in $\mathcal{S}_X$. This shows that the Wyckoff position of X is a union of infinitely many orbits if $\mathcal{S}_X$ has more than one fixed point.

Lemma

Let $\mathcal{S}_X$ be the site-symmetry group of X in $\mathcal{G}$:

(i) The points belonging to the same Wyckoff position as X are precisely the points in the orbit of X under $\mathcal{G}$ if and only if X is the only point fixed by all operations in $\mathcal{S}_X$. In this case the coordinates of a point belonging to this Wyckoff position have fixed values not depending on a parameter.

(ii) If Y is a further point fixed by all operations in $\mathcal{S}_X$ but there is no fixed point of $\mathcal{S}_X$ outside the line through X and Y, then all the points on the line through X and Y are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points on this line (with the exception of a possibly empty discrete subset of points which have a larger site-symmetry group). In this case the coordinates of a point belonging to this Wyckoff position have values depending on a single variable parameter.

(iii) If Y and Z are points fixed by all operations in $\mathcal{S}_X$ such that X, Y, Z do not lie on a line, then all the points on the plane through X, Y and Z are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points in this plane with the exception of a (possibly empty) discrete subset of lines or points which have a larger site-symmetry group. In this case the coordinates of a point belonging to this Wyckoff position have values depending on two variable parameters.

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

Figure 1.4.4.1
General-position block as given in the space-group tables for space group *P*4*bm* (100).

(iv) Only the points belonging to the general position depend on three variable parameters.

The space-group tables of Chapter 2.3 contain the following information about the Wyckoff positions of a space group $\mathcal{G}$:

Multiplicity: The Wyckoff multiplicity is the number of points in an orbit for this Wyckoff position which lie in the conventional cell. For a group with a primitive unit cell, the multiplicity for the general position equals the order of the point group of $\mathcal{G}$, while for a centred cell this is multiplied by the quotient of the volumes of the conventional cell and a primitive unit cell.

The quotient of the multiplicity for the general position by that of a special position gives the order of the site-symmetry group of the special position.

Wyckoff letter: Each Wyckoff position is labelled by a letter in alphabetical order, starting with '*a*' for a position with site-symmetry group of maximal order and ending with the highest letter (corresponding to the number of different Wyckoff positions) for the general position.

It is common to specify a Wyckoff position by its multiplicity and Wyckoff letter, *e.g.* by 4*a* for a position with multiplicity 4 and letter *a*.

Site symmetry: The point group isomorphic to the site-symmetry group is indicated by an *oriented symbol*, which is a variation of the Hermann–Mauguin point-group symbol that provides information about the orientation of the symmetry elements. The constituents of the oriented symbol are ordered according to the symmetry directions of the corresponding crystal lattice (primary, secondary and tertiary). A symmetry operation in the site-symmetry group gives rise to a symbol in the position corresponding to the direction of its geometric element. Directions for which no symmetry operation contributes to the site-symmetry group are represented by a dot in the oriented symbol.

Coordinates: Under this heading, the coordinates of the points in an orbit belonging to the Wyckoff position are given, possibly depending on one or two variable parameters (three for the general position). The points given represent the orbit up to translations from the full translational subgroup. For a space group with a centred lattice, centring vectors which are coset representatives for the translation lattice relative to the lattice spanned by the conventional basis are given at the top of the table. To obtain representatives of the orbit up to translations from the lattice spanned by the conventional basis, these centring vectors have to be added to each of the given points.

As already mentioned, the coordinates given for the general position can also be interpreted as a compact notation for the symmetry operations, specified up to translations.

The entries in the last column, the *reflection conditions*, are discussed in detail in Chapter 1.6. This column lists the conditions for the reflection indices *hkl* for which the corresponding structure factor is not systematically zero.

Examples

(1) Let $\mathcal{G}$ be the space group of type *Pbca* (61) generated by the twofold screw rotations $\{2_{001}|\frac{1}{2},0,\frac{1}{2}\}$: $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ and $\{2_{010}|0,\frac{1}{2},\frac{1}{2}\}$: $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$, the inversion $\{\bar{1}|0\}$: $\bar{x},\bar{y},\bar{z}$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$.
Applying the eight coset representatives of $\mathcal{G}$ with respect to the translation subgroup, the points in the orbit of the origin $X_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}$ that lie in the unit cell are found to be X_1, $X_2 = \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$, $X_3 = \begin{pmatrix}0\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$ and $X_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$, and the Wyckoff position to which X_1 belongs has multiplicity 4 and is labelled 4*a*.
Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_{X_1}$ has order 8/4 = 2. The inversion in the origin X_1 obviously fixes X_1, hence $\mathcal{S}_{X_1} = \{\{1|0\},\{\bar{1}|0\}\}$. The oriented symbol for the site symmetry is $\bar{1}$, indicating that the site-symmetry group is generated by an inversion.
The points X_2, X_3 and X_4 belong to the same Wyckoff position as X_1, since they lie in the orbit of X_1 and thus have conjugate site-symmetry groups.
The point $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ also has an orbit with 4 points in the unit cell, namely Y_1, $Y_2 = \begin{pmatrix}\frac{1}{2}\\0\\0\end{pmatrix}$, $Y_3 = \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$ and $Y_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$. These points therefore belong to a common Wyckoff position, namely position 4*b*. Moreover, the site-symmetry group of Y_1 is also generated by an inversion, namely the inversion $\{\bar{1}|0,0,1\}$: $\bar{x},\bar{y},\bar{z}+1$ located at Y_1 and is thus denoted by the oriented symbol $\bar{1}$.
The points X_1 and Y_1 do not belong to the same Wyckoff position, because an operation $(\boldsymbol{W},\boldsymbol{w})$ in $\mathcal{G}$ conjugates the inversion $\{\bar{1}|0,0,0\}$ in the origin to an inversion in $\boldsymbol{w}$. Since the translational parts of the operations in $\mathcal{G}$ are (up to integers) $(0,0,0)$, $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$ and $(0,\frac{1}{2},\frac{1}{2})$, an inversion in $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ can not be obtained by conjugation with operations from $\mathcal{G}$.

(2) Let $\mathcal{G}$ be the space group of type *P*4*bm* (100) generated by the fourfold rotation $\{4^+|0\}$: $\bar{y},x,z$, the glide reflection (of *b* type) $\{m_{100}|\frac{1}{2},\frac{1}{2},0\}$: $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$. The general-position coordinate triplets are shown in Fig. 1.4.4.1
From this information, the coordinates for the orbit of a specific point X in a special position can be derived by simply inserting the coordinates of X into the general-

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.

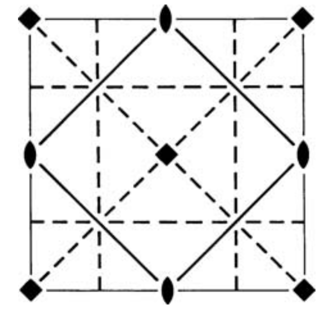

Figure 1.4.4.2
Symmetry-element diagram for the space group *P*4*bm* (100) for the orthogonal projection along [001].

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