*International Tables for Crystallography* (2016). Vol. A, Figure 1.4.4.1, p. 63.



**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-