International Tables for Crystallography (2016). Vol. A, Figure 1.4.4.3, p. 65.

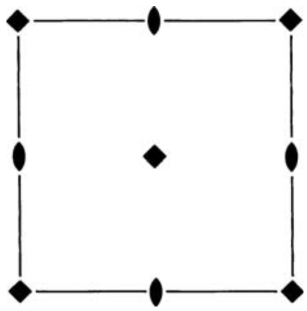

Figure 1.4.4.3
Symmetry-element diagram for the space group *P*4 (75) for the orthogonal projection along [001].

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

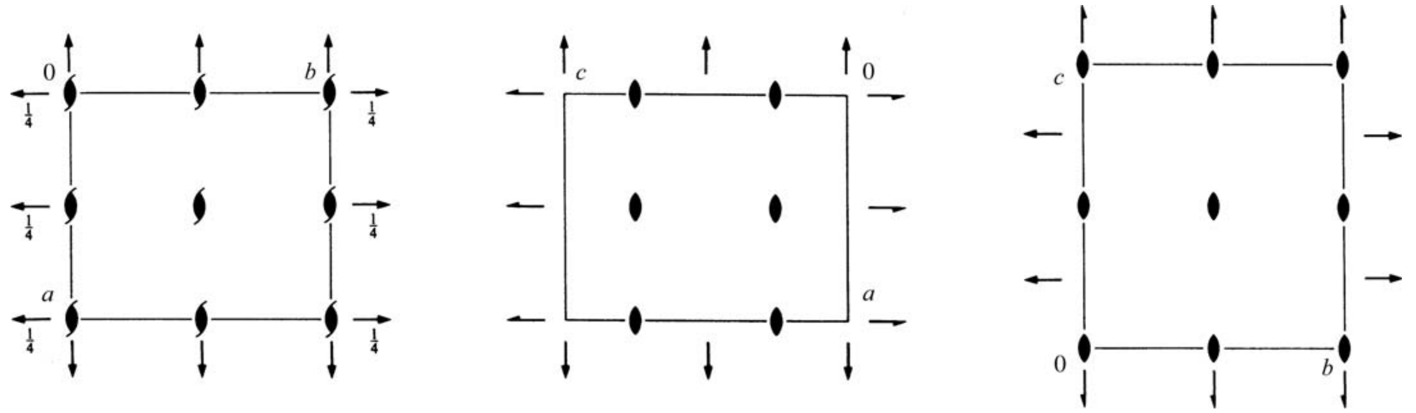

Figure 1.4.4.4
Symmetry-element diagrams for the space group $P222_1$ (17) for orthogonal projections along [001], [010], [100] (left to right).

