International Tables for Crystallography (2016). Vol. A, Section 3.4.1.3, pp. 793–794.

Accordingly, all orbits of a certain Wyckoff position belong to the same Wyckoff set. The assignment of orbits to Wyckoff sets, therefore, also defines an equivalence relation on the Wyckoff positions of a space group. The Wyckoff sets of the space groups were first tabulated by Koch & Fischer (1975).

Example

In space group *Pmna*, the site-symmetry groups of the points 0.2, 0, 0 and 0.2, 0.5, 0 are {1; 2 *x*, 0, 0} and {1; 2 *x*, $\frac{1}{2}$, 0}. There is no symmetry operation from *Pmna* that maps these site-symmetry groups onto another by conjugation and hence the two corresponding orbits do not belong to the same Wyckoff position of *Pmna*. The Euclidian (and affine) normalizer of *Pmna* is a space group of type *Pmmm* with half the lattice parameters compared with those of *Pmna* (*cf.* Chapter 3.5). It contains *e.g.* the twofold rotation 2 *x*, $\frac{1}{4}$, 0 that maps by conjugation the two site-symmetry groups onto another and also the two axes in the space-group diagram. Therefore, the two orbits belong to the same Wyckoff set even though they belong to the different Wyckoff positions 4*e* and 4*f*.

In analogy to the transition from a single space group to its type, it seems desirable to transfer also the terms 'Wyckoff position' and 'Wyckoff set' to the whole space-group type. For Wyckoff positions, however, such a generalization is not possible: two space groups of the same type can be mapped onto each other by infinitely many isomorphisms or affine mappings. Each isomorphism results in a unique relation between the Wyckoff positions of the two groups, but different isomorphisms may give rise to different relations so that the Wyckoff positions of the same Wyckoff set change their roles.

Such ambiguities, however, cannot occur for Wyckoff sets, because all Wyckoff sets of a certain space group differ in their group-theoretical relations to that group. Therefore, Wyckoff sets may be classified as follows:

Two Wyckoff sets stemming from space groups of the same type belong to the same *type of Wyckoff set* if and only if they are related by an isomorphism (affine mapping) of the two space groups (German: *Klasse von Konfigurationslagen*, *cf.* Fischer & Koch, 1974*a*; Koch & Fischer, 1975). The 219 types of space group in $\mathbb{E}^3$ give rise to 1128 types of Wyckoff set.

Example

Take, in a particular space group of type *P*4/*mmm*, the Wyckoff position 4*l* *x*, 0, 0. The points of each corresponding orbit form squares that replace the points of the tetragonal primitive point lattice of Wyckoff position 1*a*. For all conceivable orbits of 4*l*, the squares have the same orientation, but their edges differ in their lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the orbits of the Wyckoff positions 4*m*, 4*n* and 4*o*, respectively, in the same space group. The four Wyckoff positions 4*l* to 4*o*, all with site symmetry *m*2*m*., make up a Wyckoff set (*cf.* Table 3.4.3.3). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type *P*4/*mmm* is mapped onto another space group of the same type, the Wyckoff set 4*l* to 4*o* as a whole is transformed to 4*l* to 4*o*. The individual Wyckoff positions may be interchanged, however, because of the different possible choices for the origin in each individual space group of type *P*4/*mmm*. All the Wyckoff sets 4*l* to 4*o* stemming from all different space groups of type *P*4/*mmm* constitute together a type of Wyckoff set.

3.4.1.3. Point configurations and lattice complexes, reference symbols

For the comparison of crystal structures belonging to different types, another kind of equivalence relationship between crystallographic orbits may be useful:

One may consider the set of points belonging to a certain orbit without paying attention to the generating space group of the orbit. Such a bare set of points is called a *point configuration*. Two crystallographic orbits are called *configuration equivalent* if their point configurations are identical.

This definition uniquely assigns orbits to point configurations, but not *vice versa*.

Example

Let us consider a certain space group of type $Pm\bar{3}m$ with lattice vectors **a**, **b**, **c** together with two of its non-maximal subgroups, namely $Fm\bar{3}$ with index 4 and *P*432 with index 16, both with lattice vectors 2**a**, 2**b**, 2**c**. The orbit of $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ belongs to Wyckoff position 1*b* of $Pm\bar{3}m$ (site symmetry $m\bar{3}m$), and the corresponding set of points, its point configuration, forms a primitive cubic point lattice. As both subgroups have doubled unit-cell edges, the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ turns to $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. The respective orbits belong to Wyckoff position 8*c* of $Fm\bar{3}$ (site symmetry 23.) and to 8*g* of *P*432 (site symmetry .3.), and both correspond to the original point configuration. Therefore, the three orbits $Pm\bar{3}m$ 1*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, $Fm\bar{3}$ 8*c* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and *P*432 8*g* *x*, *x*, *x* with $x = \frac{1}{4}$ are configuration equivalent (together with several other orbits from certain other subgroups of $Pm\bar{3}m$). They all give rise to one and the same point configuration, a specific primitive cubic lattice of points. The generating space group, however, cannot be identified just by looking at the point configuration.

The *eigensymmetry* of a point configuration is the most comprehensive space group that maps this point configuration onto itself. Accordingly, exactly one crystallographic orbit out of each class of configuration-equivalent orbits stands out because its generating space group coincides with the eigensymmetry of its point configuration. In the case of the example above, this specific orbit is $Pm\bar{3}m$ 1*b* (as long as the origin of $Pm\bar{3}m$ remains unchanged).

The concept of configuration equivalence may also be applied to types of Wyckoff set: two types of Wyckoff set are *configuration equivalent* if and only if for each crystallographic orbit belonging to the first type there exists a configuration-equivalent crystallographic orbit belonging to the second type of Wyckoff set, and *vice versa*. All types of Wyckoff set differ in their crystallographic orbits, but configuration-equivalent types of Wyckoff set result in the same set of point configurations.

A *lattice complex* is the set of all point configurations that correspond to the crystallographic orbits of a certain type of Wyckoff set.

There exist 402 classes of configuration-equivalent types of Wyckoff set and, therefore, 402 lattice complexes in $\mathbb{E}^3$.

Example

Let us consider again the type of Wyckoff set *P*4/*mmm* 4*l* to 4*o* (the last example in Section 3.4.1.2). The set of all corresponding point configurations constitutes a lattice complex. Its

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point configurations may be derived as described above, but now – instead of starting from just a particular group – starting from all space groups of type $P4/mmm$ with all conceivable positions of the origins and lengths and orientations of the basis vectors. Accordingly, the point configurations may differ in their relative position in space, their orientation, and in the distances between the centres and the size of their squares.

Just as all crystal forms of a particular type may be related to different point-group types, the same lattice complex may occur in different space-group types.

Example

The lattice complex 'cubic primitive lattice' may be generated, among others, in $Pm\bar{3}m$ $1a, b$, in $Fm\bar{3}m$ $8c$ and in $Ia\bar{3}$ $8a, b$ with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ $1a, b$ leads to the same set of point configurations as $Fm\bar{3}m$ $8c$ or $Ia\bar{3}$ $8a, b$. Each point configuration of this lattice complex can be generated by a properly chosen space group of each of these space-group types.

Configuration-equivalent crystallographic orbits do not necessarily belong to configuration-equivalent types of Wyckoff set.

Example

The orbits of the types of Wyckoff set $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$ both refer to the set of all conceivable primitive cubic point lattices. Therefore, these two types of Wyckoff set are configuration equivalent and are associated with the same lattice complex. The type of Wyckoff set $P432$ $8g$ x, x, x, however, comprises apart from crystallographic orbits with $x = \frac{1}{4}$ also those with $x \neq \frac{1}{4}$. The orbits with $x = \frac{1}{4}$ refer to the same set of point configurations as $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, whereas those with $x \neq \frac{1}{4}$ give rise to point configurations with different properties. As a consequence, the type of Wyckoff set $P432$ $8g$ x, x, x is not configuration equivalent with $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, and, therefore, belongs to another lattice complex.

As this example shows, lattice complexes do not form equivalence classes of point configurations, but a certain point configuration may belong to several lattice complexes.

As each type of Wyckoff set uniquely refers to a certain lattice complex, one can also assign all corresponding Wyckoff sets, Wyckoff positions and crystallographic orbits to that lattice complex. A certain lattice complex, however, is frequently related to different types of Wyckoff set.

Among the different types of Wyckoff set belonging to a certain lattice complex, one stands out because its crystallographic orbits show the highest site symmetry. This one is called the *characteristic type of Wyckoff set* of that lattice complex, and the corresponding space-group type its *characteristic space-group type*. All other types of Wyckoff set are referred to as non-characteristic. The term 'characteristic' may also be transferred to particular Wyckoff sets out of the characteristic type. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of its characteristic type.

Different lattice complexes may have the same characteristic space-group type, but then they differ in the oriented site symmetry of their Wyckoff positions within that space-group type.

The characteristic space-group type together with the oriented site symmetry expresses the common symmetry properties of all point configurations of a lattice complex and can be used for its identification. For the purpose of *reference symbols* of lattice complexes, however, instead of the site symmetry the Wyckoff letter of one of the Wyckoff positions with that site symmetry is arbitrarily chosen, as first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Example

$Pm\bar{3}m$ is the characteristic space-group type for the lattice complex of all cubic primitive point lattices. The Wyckoff positions with the highest possible site symmetry $m\bar{3}m$ are $1a$ $0, 0, 0$ and $1b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, from which $1a$ has been chosen as the characteristic position. Thus, the reference symbol of this lattice complex is $Pm\bar{3}m$ a.

Example

$Pm\bar{3}m$ is also the characteristic space-group type for a second lattice complex that corresponds to Wyckoff position $8g$ $.3m$ x, x, x. The reference symbol for this lattice complex is $Pm\bar{3}m$ g. Each of its point configurations may be derived by replacing each point of a cubic primitive lattice by eight points arranged at the corners of a cube.

All types of Wyckoff set (together with their Wyckoff sets and Wyckoff positions) that generate, as described above, the same set of point configurations are assigned to the same lattice complex. Accordingly, the following criterion holds: two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family (*cf.* Section 1.3.4.4). Suitable transformations are translations, proper or improper rotations, isotropic or anisotropic expansions or more general affine mappings (without violation of the metric conditions for the corresponding crystal family), and all their products.

By this criterion, the Wyckoff positions of all space groups (1731 entries in the space-group tables, 1128 types of Wyckoff set) are uniquely assigned to 402 lattice complexes. This assignment was first done by Hermann in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). The corresponding information has also been given by Fischer *et al.* (1973).

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries in the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968). The complexes for the crystallographic subperiodic groups in three-dimensional space, *i.e.* for the crystallographic point groups, rod groups and layer groups, have been derived by Koch & Fischer (1978*a*).

3.4.1.4. Limiting complexes and comprehensive complexes

As has been shown above, lattice complexes define equivalence classes of orbits but not of point configurations. This property gave rise to the concept of limiting complexes and comprehensive complexes (Fischer & Koch, 1974*a*; Koch, 1974).

For morphological crystal forms an almost analogous situation exists. A certain tetragonal prism, for example, may be a general representative of the crystal form 'tetragonal prism' on the one hand or it may be a special representative of the crystal forms 'tetragonal pyramid' or 'tetragonal disphenoid' on the other hand. In the first case the generating point group may belong to the types $4/mmm$, 422, $4/m$ or $\bar{4}2m$ (with site symmetry 2 for each face), in the second case the types of the generating point group

references