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# 3.4. Lattice complexes

W. Fischer and E. Koch

## 3.4.1. The concept of lattice complexes and limiting complexes

### 3.4.1.1. Introduction

The term *lattice complex* (*Gitterkomplex*) was originally coined by P. Niggli (1919), but he used the term in an ambiguous manner. Later, Hermann (1935) modified and specified the concept of lattice complexes. The rigorous definition used in this chapter was proposed later still by Fischer & Koch (1974*a*) [*cf.* also Koch & Fischer (1978*a*)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at around the same time.

In crystal structures belonging to different structure types and showing different space-group symmetries, some of the atoms may have the same relative locations (*e.g.* Cl in CsCl and F in $CaF_2$). The concept of *lattice complexes* can be used to reveal relationships between such crystal structures even if their space groups belong to different types.

The terms 'point configuration' (Fischer & Koch, 1974*a*) and 'crystallographic orbit' (Matsumoto & Wondratschek, 1979) have frequently been used as synonyms for sets of points in three-dimensional space $\mathbb{E}^3$ that are equivalent with respect to a space group $\mathcal{G}$. Such sets of points may be classified in two different ways: (1) according to the concept of lattice complexes (German: *Gitterkomplexe*) and of limiting complexes, which goes back to Hermann (1935) and has been defined more strictly by Fischer & Koch (1974*a*); (2) according to the concept of types of crystallographic orbits and of non-characteristic orbits introduced by Wondratschek (1976). As the two approaches[1] are strongly related but not identical, the classes originating from the two concepts will be compared and the differences worked out.

Both terms, 'point configuration' and 'crystallographic orbit', have been used with two slightly different meanings: (1) for sets of points that are equivalent with respect to a given space group, *i.e.* in the mathematical sense of 'orbit'; (2) for such sets of points, but detached from their generating space groups. The second meaning is referred to, for example, if one speaks only of a primitive cubic point lattice. As within both concepts both meanings are required, one has to distinguish between them. In the following, therefore, the term 'crystallographic orbit' is restricted to the first meaning and the term 'point configuration' is restricted to the second meaning.

### 3.4.1.2. Crystallographic orbits, Wyckoff positions, Wyckoff sets and types of Wyckoff set

In mathematics, an orbit is a very general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group (*cf.* Section 1.1.7). In fact, orbits are always present in crystallography where equivalence classes are defined by means of a group action (*e.g.* a space-group type is the orbit of a space group in the set of all space groups under the action of the affine group). In the present context, however, the term (crystallographic) orbit will be used in a much more restricted sense, as proposed by Wondratschek (1976):

From any point of $\mathbb{E}^3$, the symmetry operations of a given space group $\mathcal{G}$ generate an infinite set of symmetry-equivalent points, called a *crystallographic orbit with respect to* $\mathcal{G}$ or, for short, a *crystallographic orbit* (*cf.* Section 1.4.4). The space group $\mathcal{G}$ is called the *generating space group* of the orbit.

Each point of a crystallographic orbit defines uniquely a largest finite subgroup of $\mathcal{G}$, which maps that point onto itself, its *site-symmetry group* (*cf.* Section 1.4.4). Site-symmetry groups that belong to different points out of the same crystallographic orbit are conjugate subgroups of $\mathcal{G}$.

*Example*

The points $x, 0, 0$ and $-x+\frac{1}{2}, 0, \frac{1}{2}$; $-x, 0, 0$ and $x+\frac{1}{2}, 0, \frac{1}{2}$ form an orbit of a given space group *Pmna* together with the infinitely many other points that can be generated from the first four by the translations of *Pmna*. The site-symmetry group 2.. of each such point consists of the identity operation 1 and of a twofold rotation. The position of the twofold axis can easily be read from the corresponding coordinate triplet. The site-symmetry groups of the first two points are $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$, respectively. They can be mapped onto another by conjugation *e.g.* with the glide reflection $a\ x, y, \frac{1}{4}$ of *Pmna*. This glide reflection also interchanges the two twofold axes as can easily be learned by inspecting the space-group diagram.

The crystallographic orbits of a given space group $\mathcal{G}$ subdivide the set of all points of $\mathbb{E}^3$ into equivalence classes. It is also possible, however, to define equivalence of orbits on the set of all crystallographic orbits of $\mathcal{G}$:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same Wyckoff position (*cf.* Section 1.4.4) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of $\mathcal{G}$.[2]

*Example*

The points 0.2, 0, 0 and 0.1, 0, 0.5 belong to different orbits of a given space group *Pmna*. Their site-symmetry groups $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$ are conjugate subgroups of *Pmna* (*cf.* the previous example). Therefore, the two orbits belong to the same Wyckoff position of *Pmna*, namely to 4*e*.

The following definition results in a coarser classification of crystallographic orbits:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same *Wyckoff set* (German: *Konfigurationslage*, *cf.* Fischer & Koch, 1974*a*) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of the affine normalizer of $\mathcal{G}$ (*cf.* Section 1.4.4.3).[3]

[1] The following articles are also related to these topics: Engel (1983); Engel *et al.* (1984); Fischer *et al.* (1973); Fischer & Koch (1978, 1983); Koch (1974); Koch & Fischer (1975, 1978*a*, 1985); Steinmann (1984); Wondratschek (1980).

[2] Instead of conjugation by symmetry operations of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used inner automorphisms of $\mathcal{G}$.

[3] Instead of conjugation by elements of the affine normalizer of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used automorphisms of $\mathcal{G}$.

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 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 $Pm\bar{3}m$ 1$a, b$, in $Fm\bar{3}m$ 8$c$ and in $Ia\bar{3}$ 8$a, b$ with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ 1$a, b$ leads to the same set of point configurations as $Fm\bar{3}m$ 8$c$ or $Ia\bar{3}$ 8$a, b$. 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 $Pm\bar{3}m$ 1$a, b$ and $Fm\bar{3}$ 8$c$ 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 $P432$ 8$g$ $x, x, x$, 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 $Pm\bar{3}m$ 1$a, b$ and $Fm\bar{3}$ 8$c$, whereas those with $x \neq \frac{1}{4}$ give rise to point configurations with different properties. As a consequence, the type of Wyckoff set $P432$ 8$g$ $x, x, x$ is not configuration equivalent with $Pm\bar{3}m$ 1$a, b$ and $Fm\bar{3}$ 8$c$, 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 1$a$ 0, 0, 0 and 1$b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, from which 1$a$ 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 8$g$ $.3m$ $x, x, x$. 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 are $4mm$ or $4$ and $\bar{4}2m$ (site symmetry $m$) or $\bar{4}$, respectively. The crystal form 'tetragonal prism' is a limiting form of both crystal forms 'tetragonal pyramid' and 'tetragonal disphenoid'.

If a first lattice complex forms a true subset of a second one, *i.e.* if each point configuration of the first lattice complex also belongs to the second one, then the first one is called a *limiting complex* of the second one and the second complex is called a *comprehensive complex* of the first one (*cf.* Koch & Fischer, 1985).

*Example*

The cubic lattice complex $I\bar{4}3d$ 16$c$ $x, x, x$ involves two limiting complexes, namely $Im\bar{3}m$ 2$a$ $0, 0, 0$ and $Ia\bar{3}d$ 16$b$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$. The orbits from $I\bar{4}3d$ 16$c$ with $x = 0$ and from $Im\bar{3}m$ 2$a$ are configuration equivalent, and so are the orbits from $I\bar{4}3d$ 16$c$ with $x = \frac{1}{8}$ and from $Ia\bar{3}d$ 16$b$.

*Example*

The tetragonal lattice complex $I4_1/amd$ 4$a$ is a comprehensive complex of the cubic complex $Fd\bar{3}m$ 8$a$. Each orbit of $Fd\bar{3}m$ 8$a$ is configuration equivalent to a crystallographic orbit of a special space group of type $I4_1/amd$ with axial ratio $c/a = (2)^{1/2}$.

Furthermore, two lattice complexes without a limiting-complex relationship may have a non-empty intersection. Then the point configurations of the intersection result in one or, in very exceptional cases, in two or more other lattice complexes (*cf.* Koch, 1974).

*Example*

The intersection of the two lattice complexes $Im\bar{3}$ 24$g$ and $I\bar{4}3m$ 24$g$ consists of all point configurations belonging to $Im\bar{3}m$ 24$h$, *i.e.* each point configuration out of this intersection refers to an orbit from $Im\bar{3}m$ 24$h$ $0, x, x$ and, in addition, to an orbit from $Im\bar{3}$ 24$g$ $0, y, z$ with $y = z$ and to another one from $I\bar{4}3m$ 24$g$ $x, x, z$ with $z = 0$.

*Example*

The intersection of the trivariant lattice complexes $Fm\bar{3}c$ 192$j$ and $P432$ 24$k$ consists of two bivariant limiting complexes, namely of $Pm\bar{3}m$ 24$k$ $0, y, z$ and of $Pm\bar{3}m$ 24$m$ $x, x, z$.

Each point configuration of a given lattice complex is uniquely related to two space groups: (1) the space group that reflects its eigensymmetry, and (2) a space group that belongs to the characteristic space-group type of the lattice complex under consideration. In most cases the two groups coincide. Only when the point configuration under consideration belongs to a limiting complex is the first group a proper supergroup of the second one.

Complete lists of the limiting complexes of all lattice complexes are not available. Koch (1974) derived the limiting complexes of the cubic lattice complexes. The limiting complexes that refer to specialized coordinate parameters may be derived from a table by Engel *et al.* (1984), who listed the respective non-characteristic orbits for all space-group types. The limiting complexes of the tetragonal and trigonal lattice complexes that are due to metrical specializations are tabulated by Koch & Fischer (2003) and by Koch & Sowa (2005), respectively.

Fischer & Koch (1978) tabulated the limiting complexes for the crystallographic point groups, rod groups and layer groups. As each type of plane group uniquely corresponds to a certain type of isomorphic layer group, information on the limiting complexes of the lattice complexes of the plane groups may easily be extracted from the respective table for the layer groups. This information may also be taken from a list of the non-characteristic orbits of the plane groups by Matsumoto & Wondratschek (1987).

### 3.4.1.5. Additional properties of lattice complexes

*3.4.1.5.1. The degrees of freedom*

Each Wyckoff position shows a certain number of coordinate parameters that can be varied independently. For most lattice complexes, this number is the same for any of its Wyckoff positions. For the lattice complex with characteristic Wyckoff position $Pm\bar{3}$ 12$j$ $m..$ $0, y, z$, for instance, this number is two. The lattice complex has two degrees of freedom. If, however, the variation of a certain coordinate corresponds to a shift of the point configuration as a whole, the lattice complex has fewer degrees of freedom than the Wyckoff position that is being considered. Therefore, $I4_1$ 8$b$ $x, y, z$ is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8$b$ itself has three coordinate parameters that can be varied independently. The lattice complex $P4/m$ $j$ has two degrees of freedom and refers to Wyckoff positions with two as well as with three independent coordinate parameters, namely to $P4/m$ 4$j$ $m..$ $x, y, 0$ and to $P4$ 4$d$ 1 $x, y, z$.

According to its number of degrees of freedom, a lattice complex is called *invariant*, *univariant*, *bivariant* or *trivariant*. In total, there exist 402 lattice complexes, 36 of which are invariant, 106 univariant, 105 bivariant and 155 trivariant. The 30 plane lattice complexes are made up of 7 invariant, 10 univariant and 13 bivariant ones.

Most of the invariant and univariant lattice complexes correspond to several types of Wyckoff set. In contrast to that, only one type of Wyckoff set can belong to each trivariant lattice complex. A bivariant lattice complex may either correspond to one type of Wyckoff set (*e.g.* $Pm\bar{3}$ $j$) or to two types ($P4$ $d$, for example, belongs to the lattice complex with the characteristic Wyckoff position $P4/m$ $j$).

*3.4.1.5.2. Weissenberg complexes*

Depending on their site-symmetry groups, two kinds of Wyckoff position may be distinguished:

(i) The site-symmetry group of any point is a proper subgroup of another site-symmetry group from the same space group. Then the Wyckoff position contains, among others, orbits where suitably chosen points may be infinitely close together.

*Example*

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm$ 4$j$ $m.2m$ $x, x, 0$ may be imagined as squares of four points surrounding the points of a tetragonal primitive lattice. For $x \to 0$, the squares become infinitesimally small. Orbits with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to Wyckoff position $P4/mmm$ 1$a$.

(ii) The site-symmetry group of every point belonging to the Wyckoff position under consideration is not a proper subgroup of any other site-symmetry group from the same space group.

*Example*

In $Pmma$, there does not exist a site-symmetry group that is a proper supergroup of $mm2$, the site symmetry of Wyckoff position $Pmma$ 2$e$ $\frac{1}{4}, 0, z$. As a consequence, the

**Table 3.4.1.1**
Reference symbols of the 31 Weissenberg complexes with $f \geq 1$ degrees of freedom in $\mathbb{E}^3$

| Weissenberg complex | $f$ | Weissenberg complex | $f$ |
|---|---|---|---|
| $P2_1/m\ e$ | 2 | $I\bar{4}2d\ d$ | 1 |
| $P2/c\ e$ | 1 | $P4/nmm\ c$ | 1 |
| $C2/c\ e$ | 1 | $I4_1/acd\ e$ | 1 |
| $P2_12_12_1\ a$ | 3 | $P3_2\ a$ | 2 |
| $Pmma\ e$ | 1 | $P3_212\ a$ | 1 |
| $Pbcm\ d$ | 2 | $P3_221\ a$ | 1 |
| $Pmmn\ a$ | 1 | $P\bar{3}m1\ d$ | 1 |
| $Pnma\ c$ | 2 | $P6_1\ a$ | 2 |
| $Cmcm\ c$ | 1 | $P6_122\ a$ | 1 |
| $Cmme\ g$ | 1 | $P6_122\ b$ | 1 |
| $Imma\ e$ | 1 | $P2_13\ a$ | 1 |
| $P4_3\ a$ | 2 | $I2_13\ a$ | 1 |
| $P4_322\ a$ | 1 | $I2_13\ b$ | 1 |
| $P4_322\ c$ | 1 | $Ia\bar{3}\ d$ | 1 |
| $P4_32_12\ a$ | 1 | $I\bar{4}3d\ c$ | 1 |
| $I4_122\ f$ | 1 | | |

distance between any two symmetry-equivalent points belonging to *Pmma e* cannot become shorter than the minimum of $\frac{1}{2}a$, $b$ and $c$.

A lattice complex refers either to Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are related to Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes without point configurations with infinitesimally short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes were called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. The other 31 Weissenberg complexes with degrees of freedom (24 univariant, 6 bivariant, 1 trivariant) are compiled in Table 3.4.1.1. They have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family (see also Section 3.4.3.1.3).

*Example*

The Weissenberg complex *Pmma* 2*e* $\frac{1}{4}, 0, z$ is a comprehensive complex of *Pmmm a* and of *Cmmm a*. Within the characteristic Wyckoff position, $\frac{1}{4}, 0, 0$ refers to *Pmmm a* and $\frac{1}{4}, 0, \frac{1}{4}$ to *Cmmm a*.

Apart from the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex *p*2*mg c*.

## 3.4.2. The concept of characteristic and non-characteristic orbits, comparison with the lattice-complex concept

### 3.4.2.1. Definitions

The generating space group of any crystallographic orbit may be compared with the eigensymmetry of its point configuration. If both groups coincide, the orbit is called a *characteristic crystallographic orbit*, otherwise it is named a *non-characteristic crystallographic orbit* (Wondratschek, 1976; Engel *et al.*, 1984; see also Section 1.1.7). If the eigensymmetry group contains additional translations in comparison with those of the generating space group, the term *extraordinary orbit* is used (*cf.* also Matsumoto & Wondratschek, 1979). Each class of configuration-equivalent orbits contains exactly one characteristic crystallographic orbit.

The set of all point configurations in $\mathbb{E}^3$ can be divided into 402 equivalence classes by means of their eigensymmetry: two point configurations belong to the same *symmetry type of point configuration* if and only if their characteristic crystallographic orbits belong to the same type of Wyckoff set.

As each crystallographic orbit is uniquely related to a certain point configuration, each equivalence relationship on the set of all point configurations also implies an equivalence relationship on the set of all crystallographic orbits: two crystallographic orbits are assigned to the same *orbit type* (*cf.* also Engel *et al.*, 1984) if and only if the corresponding point configurations belong to the same symmetry type.

In contrast to lattice complexes, neither symmetry types of point configuration nor orbit types can be used to define equivalence relations on Wyckoff positions, Wyckoff sets or types of Wyckoff set. Two crystallographic orbits coming from the same Wyckoff position belong to different orbit types, if – owing to special coordinate values – they differ in the eigensymmetry of their point configurations. Furthermore, two crystallographic orbits with the same coordinate description, but stemming from different space groups of the same type, may belong to different orbit types because of a specialization of the metrical parameters.

*Example*

The eigensymmetry of orbits from Wyckoff position $P\bar{4}3m$ 4*e* $x, x, x$ with $x = \frac{1}{4}$ or $x = \frac{3}{4}$ is enhanced to $Fm\bar{3}m$ 4*a*, *b* and hence they belong to a different orbit type to those with $x \neq \frac{1}{4}, \frac{3}{4}$.

*Example*

In general, an orbit belonging to the type of Wyckoff set *I*4/*m* 2*a*, *b* corresponds to a point configuration with eigensymmetry *I*4/*mmm* 2*a*, *b*. If, however, the space group *I*4/*m* has specialized metrical parameters, *e.g.* $c/a = 1$ or $c/a = 2^{1/2}$, then the eigensymmetry of the point configuration is enhanced to $Im\bar{3}m$ 2*a* or $Fm\bar{3}m$ 4*a*, *b*, respectively.

### 3.4.2.2. Comparison of the concepts of lattice complexes and orbit types

It is the common intention of the lattice-complex and the orbit-type concepts to subdivide the point configurations and crystallographic orbits in $\mathbb{E}^3$ into subsets with certain common properties. With only a few exceptions, the two concepts result in different subsets. As similar but not identical symmetry considerations are used, each lattice complex is uniquely related to a certain symmetry type of point configuration and to a certain orbit type, and *vice versa*. Therefore, the two concepts result in the same number of subsets: there exist 402 lattice complexes and 402 symmetry types of point configuration and orbit types. The differences between the subsets are caused by the different properties of the point configurations and crystallographic orbits used for the classifications (*cf.* also Koch & Fischer, 1985).

The concept of orbit types is entirely based on the eigensymmetry of the particular point configurations: a crystallographic orbit is regarded as an isolated entity, *i.e.* detached from its Wyckoff position and its type of Wyckoff set. On the contrary, lattice complexes result from a hierarchy of classifications of crystallographic orbits into Wyckoff positions, Wyckoff sets, types of Wyckoff set and classes of configuration-equivalent types of


references