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

Example

The tetragonal lattice complex $I4_1/amd$ 4a is a comprehensive complex of the cubic complex $Fd\bar{3}m$ 8a. Each orbit of $Fd\bar{3}m$ 8a 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 $Im\bar{3}$ 24g and $I\bar{4}3m$ 24g consists of all point configurations belonging to $Im\bar{3}m$ 24h, *i.e.* each point configuration out of this intersection refers to an orbit from $Im\bar{3}m$ 24h $0, x, x$ and, in addition, to an orbit from $Im\bar{3}$ 24g $0, y, z$ with $y = z$ and to another one from $I\bar{4}3m$ 24g x, x, z with $z = 0$.

Example

The intersection of the trivariant lattice complexes $Fm\bar{3}c$ 192j and $P432$ 24k consists of two bivariant limiting complexes, namely of $Pm\bar{3}m$ 24k $0, y, z$ and of $Pm\bar{3}m$ 24m 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 $Pm\bar{3}$ 12j $m..$ $0, y, z$, 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, $I4_1$ 8b x, y, z is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8b 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 $P4/m$ 4j $m..$ $x, y, 0$ and to $P4$ 4d 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 $P4/mmm$ 4j $m.2m$ $x, x, 0$ 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 $P4/mmm$ 1a.

(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 $Pmma$ 2e $\frac{1}{4}, 0, z$. 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