International Tables for Crystallography (2016). Vol. A, Section 3.4.2, pp. 796–798.

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* $2e\ \frac{1}{4}, 0, z$ 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 *p2mg 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 $P\bar{4}3m$ $4e\ x, x, x$ with $x = \frac{1}{4}$ or $x = \frac{3}{4}$ is enhanced to $Fm\bar{3}m$ $4a, b$ 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 $I4/m$ $2a, b$ corresponds to a point configuration with eigensymmetry $I4/mmm$ $2a, b$. If, however, the space group $I4/m$ 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 $Im\bar{3}m$ $2a$ or $Fm\bar{3}m$ $4a, b$, 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

Table 3.4.2.1
Reference symbols of the 28 lattice complexes with $f \geq 1$ degrees of freedom without any limiting complex

Lattice complex	f	Lattice complex	f
$P4/mmm$ l	1	$Pm\bar{3}n$ g	1
$P4_2/mmc$ j	1	$Pm\bar{3}n$ j	1
$I4/mmm$ i	1	$Pn\bar{3}m$ e	1
$P6_222$ g	1	$Pn\bar{3}m$ i	1
$P6/mmm$ l	1	$Fm\bar{3}m$ f	1
$P6/mmm$ p	2	$Fm\bar{3}m$ h	1
$P4_232$ k	1	$Fd\bar{3}m$ g	2
$I432$ i	1	$Im\bar{3}m$ e	1
$I4_132$ h	1	$Im\bar{3}m$ f	1
$I4_132$ i	3	$Im\bar{3}m$ g	1
$Pm\bar{3}m$ e	1	$Im\bar{3}m$ i	1
$Pm\bar{3}m$ i	1	$Im\bar{3}m$ j	2
$Pm\bar{3}m$ k	2	$Im\bar{3}m$ l	3
$Pm\bar{3}m$ m	2	$Ia\bar{3}d$ e	1

Wyckoff set, *i.e.* a crystallographic orbit is always considered as being embedded in its type of Wyckoff set, and the eigensymmetry of a particular point configuration is disregarded. The differences between the two concepts become clear if limiting complexes are considered.

Forty-nine lattice complexes without any limiting complex exist (*cf.* Table 3.4.2.1). They coincide completely with the corresponding symmetry types of point configurations. As can be extracted from the tables by Engel *et al.* (1984) there exist 15 additional lattice complexes without limiting complexes due to specialized coordinates. For fundamental reasons, no cubic or hexagonal complexes allow any metrical specialization.

Example

The lattice complex $P\bar{1}$ a of all triclinic point lattices includes as limiting complexes the 13 other lattice complexes that refer to Bravais lattices. Hence the crystallographic orbits of $P\bar{1}$ a belong to 14 different orbit types.

Example

The lattice complex $Fddd$ a of all orthorhombic diamond patterns includes as limiting complexes those of the tetragonal and the cubic diamond patterns $I4_1/amd$ a and $Fd\bar{3}m$ a, respectively. The orbits of $Fddd$ a with specialized metric, therefore, belong to the orbit types $I4_1/amd$ a or $Fd\bar{3}m$ a.

353 lattice complexes comprise at least one limiting complex. Each of them includes additional point configurations in comparison to the corresponding symmetry type of point configuration (and orbit type), namely those belonging to the limiting complex.

Example

Lattice complex $Im\bar{3}$ $24g$ $0, y, z$ comprises for $y = z$ the limiting complex $Im\bar{3}m$ $24h$, and for $y = z = \frac{1}{4}$ the limiting complex $Pm\bar{3}m$ $3c$. The corresponding orbits with $y = z$ and $y = z = \frac{1}{4}$ do not belong to orbit type $Im\bar{3}$ $24g$.

Example

$P4/mmm$ $8r$ x, x, z comprises for $z = \frac{1}{4}$ the limiting complex $P4/mmm$ $4j$, for $x = \frac{1}{4}$ the limiting complex $P4/mmm$ $2g$, for $x = z = \frac{1}{4}$ the limiting complex $P4/mmm$ $1a$, for $a = c$ and $x = z$ the limiting complex $Pm\bar{3}m$ $8g$, and for $a = c$ and $x = z = \frac{1}{4}$ the limiting complex $Pm\bar{3}m$ $1a$. Again, none of the corresponding orbits belong to orbit type $P4/mmm$ $8r$.

The comparison of an orbit type with its corresponding lattice complex is more intricate. Again, the concept of limiting complexes and comprehensive complexes elucidates the interrelation.

Let A be a lattice complex with a limiting complex B and a comprehensive complex C. The respective orbit types will also be designated A, B and C (*e.g.* $A = Im\bar{3}m$ $24h$ $0, x, x$; $B = Pm\bar{3}m$ $3c, d$ $0, \frac{1}{2}, \frac{1}{2}$, $\frac{1}{2}, 0, 0$; $C = Im\bar{3}$ $24g$ $0, y, z$). Then a crystallographic orbit from a Wyckoff position of lattice complex A belongs to orbit type A only if it does not correspond to a point configuration of the limiting complex B (*i.e.* only the crystallographic orbits of $Im\bar{3}m$ $24h$ with $x \neq \frac{1}{4}$ belong to orbit type $Im\bar{3}m$ $24h$). The crystallographic orbits of lattice complex A, however, that do correspond to the limiting complex B belong to orbit type B (*i.e.* all crystallographic orbits from $Im\bar{3}m$ $24h$ with $x = \frac{1}{4}$ belong to orbit type $Pm\bar{3}m$ $3c, d$). On the contrary, those orbits that refer to lattice complex C and that happen to correspond to the limiting complex A of C belong to orbit type A instead of orbit type C. All crystallographic orbits of $Im\bar{3}$ $24g$ $0, y, z$ with $y = z$ or $y = z = \frac{1}{4}$ create point configurations of lattice complex $Im\bar{3}$ $24g$ but belong to orbit type $Im\bar{3}m$ $24h$ or $Pm\bar{3}m$ $3c, d$, respectively.

For the comparison of lattice complexes and orbit types the concept of non-characteristic orbits is less helpful than the concept of limiting complexes. In terms of lattice complexes, there exist two basically different reasons for a crystallographic orbit to be non-characteristic:

(1) The crystallographic orbit under consideration belongs to a non-characteristic type of Wyckoff set of a lattice complex. Then this orbit, together with all other orbits from its type of Wyckoff set, is non-characteristic. A characteristic crystallographic orbit necessarily stems from a characteristic Wyckoff set of a lattice complex.
(2) The crystallographic orbit under consideration stands out with respect to the eigensymmetry of its point configuration compared with the other orbits out of its type of Wyckoff sets, *i.e.* it corresponds to a limiting complex. Then this orbit, together with all other orbits referring to that limiting complex, is non-characteristic.

As a consequence, three kinds of non-characteristic orbits may be distinguished:

(1) those that belong to a non-characteristic Wyckoff set, but do not correspond to a limiting complex, *e.g.* all orbits from $Pm\bar{3}$ $6e$ to h;
(2) those that belong to a characteristic Wyckoff set, but correspond to a limiting complex, *e.g.* $Pm\bar{3}m$ $8g$ x, x, x with $x = \frac{1}{4}$ or $P4/mmm$ $1a, b$ with $a = c$;
(3) those that belong to a non-characteristic Wyckoff set and, in addition, correspond to a limiting complex, *e.g.* $Pm\bar{3}$ $8i$ x, x, x with $x = \frac{1}{4}$.

As these considerations illustrate, limiting complexes and non-characteristic orbits do not coincide and a statement by Engel (1983) proposing this correspondence, therefore, is not correct.

The concept of lattice complexes and limiting complexes on the one hand and of orbit types and non-characteristic orbits on the other hand are complementary in a certain sense: it is possible to derive all orbit types and all non-characteristic orbits from the complete knowledge of lattice complexes and limiting complexes and *vice versa*.

Engel *et al.* (1984) enumerated for all space-group types those non-characteristic orbits that refer to special coordinates, but they excluded all further ones that are based on specialized metrical parameters of the generating space groups or on the simultaneous specialization of metrical and coordinate parameters. A computer program which enables the determination of non-characteristic orbits is now available (*NONCHAR* on the Bilbao Crystallographic Server at http://www.cryst.ehu.es). Lawrenson & Wondratschek (1976) listed the extraordinary orbits of the plane groups, and Matsumoto & Wondratschek (1987) listed the non-characteristic orbits of the plane groups.

The special, but not exceptional, case in which a non-characteristic orbit is produced only if both the coordinates *and* metric are specialized deserves extra concern. The crystallographic orbits from $R\bar{3}$ $6f$ x, y, z with $x = \frac{1}{4}, y = 0, z = \frac{1}{2}$ or $x = \frac{1}{4}, y = \frac{1}{2}, z = 0$ and with the rhombohedral angle $\alpha = 90°$ may be used as an example. The eigensymmetry of the corresponding point configurations is $Pm\bar{3}n$ $6c$, d (corresponding to the position of the Cr atoms in the crystal structure of Cr_3Si). Accordingly, the lattice complex $R\bar{3}$ f comprises $Pm\bar{3}n$ c as limiting complex. $Pm\bar{3}n$ c shows special integral reflection conditions (hkl: $h + k + l = 2n$ or $h = 2n + 1$, $k = 4n$, $l = 4n + 2$; h, k, l permutable), which of course hold for all orbits of that type, *i.e.* also for the special orbits from $R\bar{3}$ f described above. As geometrical structure factors are independent of metrical parameters, these reflection conditions are even valid for crystallographic orbits from $R\bar{3}$ f with $a \neq 90°$ if the coordinates are restricted to $\frac{1}{4}, 0, \frac{1}{2}$ or to $\frac{1}{4}, \frac{1}{2}, 0$.

In general, the following statement holds: if a lattice complex causes special reflection conditions then exactly these conditions are also valid for any crystallographic orbit that refers to a comprehensive complex of that lattice complex if, in addition, this crystallographic orbit may be described by the same coordinate triplets as an orbit of the lattice complex under consideration.

3.4.3. Descriptive lattice-complex symbols and the assignment of Wyckoff positions to lattice complexes

3.4.3.1. Descriptive symbols

3.4.3.1.1. Introduction

For the study of relations between crystal structures, lattice-complex symbols are desirable that show as many relations between point configurations as possible. To this end, Hermann (1960) derived descriptive lattice-complex symbols that were further developed by Donnay *et al.* (1966) and completed by Fischer *et al.* (1973). These symbols describe the arrangements of the points in the point configurations and refer directly to the coordinate descriptions of the Wyckoff positions. Since a lattice complex, in general, contains Wyckoff positions with different coordinate descriptions, it may be represented by several different descriptive symbols. The symbols are further affected by the settings of the space group. The present section is restricted to the fundamental features of the descriptive symbols. Details have been described by Fischer *et al.* (1973). Tables 3.4.3.2 and 3.4.3.3 give for each Wyckoff position of a plane group or a space group, respectively, the multiplicity, the Wyckoff letter, the oriented site symmetry, the reference symbol of the corresponding lattice complex and the descriptive symbol.[4] The comparatively short descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

[4] Some of the descriptive symbols listed in Table 3.4.3.3 differ slightly from those derived by Fischer *et al.* (1973) and used in editions of *International Tables for Crystallography* Volume A before 2002.

Table 3.4.3.1
Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position

Descriptive symbol	Crystal family	Characteristic Wyckoff position
C	o	$Cmmm$ a
	m	$C2/m$ a
D	c	$Fd\bar{3}m$ a
	o	$Fddd$ a
^{v}D	t	$I4_1/amd$ a
E	h	$P6_3/mmc$ c
F	c	$Fm\bar{3}m$ a
	o	$Fmmm$ a
G	h	$P6/mmm$ c
I	c	$Im\bar{3}m$ a
	t	$I4/mmm$ a
	o	$Immm$ a
J	c	$Pm\bar{3}m$ c
J^*	c	$Im\bar{3}m$ b
M	h	$R\bar{3}m$ e
N	h	$P6/mmm$ f
P	c	$Pm\bar{3}m$ a
	h	$P6/mmm$ a
	t	$P4/mmm$ a
	o	$Pmmm$ a
	m	$P2/m$ a
	a	$P\bar{1}$ a
^{+}Q	h	$P6_222$ c
R	h	$R\bar{3}m$ a
S	c	$I\bar{4}3d$ a
S^*	c	$Ia\bar{3}d$ d
T	c	$Fd\bar{3}m$ c
	o	$Fddd$ c
^{v}T	t	$I4_1/amd$ c
^{+}V	c	$I4_132$ c
V^*	c	$Ia\bar{3}d$ c
W	c	$Pm\bar{3}n$ c
W^*	c	$Im\bar{3}m$ d
^{+}Y	c	$P4_332$ a
$^{+}Y^*$	c	$I4_132$ a
Y^{**}	c	$Ia\bar{3}d$ b

3.4.3.1.2. Invariant lattice complexes

An invariant lattice complex in its characteristic Wyckoff position is represented by a capital letter (sometimes in combination with a superscript). The first column of Table 3.4.3.1 gives a complete list of these symbols in alphabetical order. The characteristic Wyckoff positions are shown in column 3. Lattice complexes from different crystal families but with the same coordinate description for their characteristic Wyckoff positions receive the same descriptive symbol. If necessary, the crystal family may be stated explicitly by a small letter (column 2) preceding the lattice-complex symbol: *c* cubic, *t* tetragonal, *h* hexagonal, *o* orthorhombic, *m* monoclinic, *a* anorthic (triclinic).

references