3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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