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*.