*International Tables for Crystallography* (2016). Vol. A, Section 3.4.3, pp. 798–800.



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).

*Example*

$D$ is the descriptive symbol of the invariant cubic lattice complex $Fd\bar{3}m\ a$ as well as of the orthorhombic lattice complex $Fddd\ a$. The cubic lattice complex $cD$ contains – among others – the point configurations corresponding to the arrangement of carbon atoms in diamond and of silicon atoms in $\beta$-cristobalite. The orthorhombic complex $oD$ is a comprehensive complex of $cD$. It consists of all those point configurations that may be produced by orthorhombic deformations of the point configurations of $cD$.

The descriptive symbol of a non-characteristic Wyckoff position depends on the difference between the coordinate descriptions of the respective characteristic Wyckoff position and the position under consideration. Three cases may be distinguished, which may also occur in combinations.

(i) The two coordinate descriptions differ by an origin shift. Then, the respective shift vector is added as a prefix to the descriptive symbol of the characteristic Wyckoff position.

*Example*

The orthorhombic invariant lattice complex $F$ is represented in its characteristic Wyckoff position $Fmmm\ a$ by the coordinate triplets $0, 0, 0,\ \frac{1}{2}, \frac{1}{2}, 0,\ 0, \frac{1}{2}, \frac{1}{2}$ and $\frac{1}{2}, 0, \frac{1}{2}$. In $Pnnn\ e$ (origin choice 1), it is described by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4},\ \frac{3}{4}, \frac{3}{4}, \frac{1}{4},\ \frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ and $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ and, therefore, receives the descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}F$.

(ii) The multiplicity of the Wyckoff position considered is higher than that of the corresponding characteristic position. Then, the coordinate description of this Wyckoff position can be transformed into that of the characteristic position by taking shorter basis vectors. Reduction of all three basis vectors by a factor of 2 is denoted by the subscript 2 on the descriptive symbol. Reduction of one or two basis vectors by a factor of 2 is denoted by one of the subscripts $a$, $b$ or $c$ or a combination of these. The subscript $C$ means a factor of 3, $cc$ a factor of 4 and $Cc$ a factor of 6.

*Examples*

The characteristic Wyckoff position of the orthorhombic lattice complex $P$ is $Pmmm\ a$ with coordinate description $0, 0, 0$. This complex occurs also in $Pmma\ a$ with coordinate triplets $0, 0, 0,\ \frac{1}{2}, 0, 0$, and in $Pcca\ a$ with $0, 0, 0,\ 0, 0, \frac{1}{2},\ \frac{1}{2}, 0, 0,\ \frac{1}{2}, 0, \frac{1}{2}$. The corresponding descriptive symbols are $P_a$ and $P_{ac}$, respectively.

(iii) The coordinate description of a given Wyckoff position is related to that of the characteristic position by inversion or rotation of the coordinate system. Changing the superscript + into − in the descriptive symbol means that the Wyckoff position considered is mapped onto the characteristic position by an inversion through the origin, *i.e.* the two Wyckoff positions are enantiomorphic. A prime preceding the capital letter denotes that a 180° rotation is required.

*Examples*

(1) $^{+}Y^{*}$ is the descriptive symbol of the invariant lattice complex $I4_132\ a$ in its characteristic position. Wyckoff position $I4_132\ b$ with the descriptive symbol $^{-}Y^{*}$ belongs to the same lattice complex. The point configurations of $I4_132\ a$ and $I4_132\ b$ are enantiomorphic.

(2) $R$ is the descriptive symbol of the invariant lattice complex formed by all rhombohedral point lattices. Its characteristic position $R\bar{3}m\ a$ corresponds to the coordinate triplets $0, 0, 0,\ \frac{2}{3}, \frac{1}{3}, \frac{1}{3},\ \frac{1}{3}, \frac{2}{3}, \frac{2}{3}$. The same lattice complex is symbolized by $'R_c$ in the non-characteristic position $R\bar{3}c\ b$ with coordinate description $0, 0, 0,\ 0, 0, \frac{1}{2},\ \frac{2}{3}, \frac{1}{3}, \frac{1}{3},\ \frac{2}{3}, \frac{1}{3}, \frac{5}{6},\ \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{1}{3}, \frac{2}{3}, \frac{1}{6}$.

In non-characteristic Wyckoff positions, the descriptive symbols $P$ and $I$ may be replaced by $C$ and $F$, respectively (tetragonal system), $C$ by $A$ or $B$ (orthorhombic system), and $C$ by $A$, $B$, $I$ or $F$ (monoclinic system). If the lattice complexes of rhombohedral space groups are described in rhombohedral coordinate systems, the symbols $R$, $'R_c$, $M$ and $'M_c$ of the hexagonal description are replaced by $P$, $I$, $J$ and $J^*$, respectively (preceded by the letter $r$, if necessary, to distinguish them from the analogous cubic invariant lattice complexes).

*3.4.3.1.3. Lattice complexes with degrees of freedom*

The descriptive symbols of lattice complexes with degrees of freedom consist, in general, of four parts: the shift vector, the distribution symmetry, the central part and the site-set symbol. Either of the first two parts may be absent.

*Example*

$0\frac{1}{2}0$ ..2 $C4xxz$ is the descriptive symbol of the lattice complex $P4/nbm\ m$ in its characteristic position: $0\frac{1}{2}0$ is the shift vector, ..2 the distribution symmetry, $C$ the central part and $4xxz$ the site-set symbol.

Normally, the central part is the symbol of an invariant lattice complex. The shift vector and central part together should be interpreted as described in Section 3.4.3.1.2. The point configurations of the Wyckoff position being considered can be derived from that described by the central part by replacing each point by a finite set of points, the site set. All points of a site set are symmetry-equivalent under the site-symmetry group of the point that they replace. A site set is symbolized by a string of numbers and letters. The product of the numbers gives the number of points in the site set, whereas the letters supply information on the pattern formed by these points. Site sets replacing different points may be differently oriented. In this case, the distribution-symmetry part of the reference symbol shows symmetry operations that relate such site sets to one another. The orientation of the corresponding symmetry elements is indicated as in the oriented site-symmetry symbols (*cf.* Section 2.2.12). If all site sets have the same orientation, no distribution symmetry is given.

*Examples*

(1) $I4xxx$ ($I\bar{4}3m\ 8c\ x, x, x$) designates a lattice complex, the point configurations of which are composed of tetrahedra $4xxx$ in parallel orientation replacing the points of a cubic body-centred lattice $I$. The vertices of these tetrahedra are located on body diagonals.

(2) ..2 $I4xxx$ ($Pn\bar{3}m\ 8e\ x, x, x$) represents the lattice complex for which, in contrast to the first example, the tetrahedra $4xxx$ around $0, 0, 0$ and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ differ in their orientation. They are related by a twofold rotation ..2 .

(3) $00\frac{1}{4}\ P_c4x$ is the descriptive symbol of Wyckoff position $P4_2/mcm\ 8l\ x, 0, \frac{1}{4}$. Each corresponding point configuration consists of squares of points $4x$ replacing the points of a tetragonal primitive lattice $P$. In comparison with $P4x$, $00\frac{1}{4}\ P_c4x$ shows a unit-cell enlargement by $\mathbf{c}' = 2\mathbf{c}$ and a subsequent shift by $0, 0, \frac{1}{4}$.

In the case of a Weissenberg complex (*cf.* Section 3.4.1.5.2; Weissenberg, 1925; Fischer *et al.*, 1973), the central part of the descriptive symbol always consists of two (or more) symbols of invariant lattice complexes belonging to the same crystal family and forming limiting complexes of the Weissenberg complex under consideration. The shift vector then refers to the first limiting complex. The corresponding site-set symbols are distinguished by containing the number 1 as the only number, *i.e.* each site set consists of only one point.

*Example*

In $\frac{1}{4}00$ .2. $P_aB1z$ (*Pmma* 2*e* $\frac{1}{4}, 0, z$), each of the two points $\frac{1}{4}, 0, 0$ and $\frac{3}{4}, 0, 0$, represented by $\frac{1}{4}00$ $P_a$, is replaced by a site set 1*z* containing only one point, *i.e.* the points of $\frac{1}{4}00$ $P_a$ are shifted along the *z* axis. The shifts of the two points are related by a twofold rotation .2., *i.e.* are running in opposite directions. The point configurations of the two limiting complexes $P_a$ and *B* refer to the special parameter values $z = 0$ and $z = \frac{1}{4}$, respectively.

The central parts of some lattice complexes with two or three degrees of freedom are formed by the descriptive symbol of a univariant Weissenberg complex instead of that of an invariant lattice complex. This is the case only if the corresponding characteristic space-group type does not refer to a suitable invariant lattice complex.

*Example*

In $\frac{1}{4}00$ .2. $P_aB1z2y$ (*Pmma* 4*k* $\frac{1}{4}, y, z$), each of the two points $\frac{1}{4}, 0, z$ and $\frac{3}{4}, 0, \bar{z}$, represented by $\frac{1}{4}00$ .2. $P_aB1z$, is replaced by a site set 2*y* of two points forming a dumbbell. These dumbbells are oriented parallel to the *y* axis.

The symbol of a non-characteristic Wyckoff position is deduced from that of the characteristic position. The four parts of the descriptive symbol are subjected to the transformation necessary to map the characteristic Wyckoff position onto the Wyckoff position under consideration.

*Example*

The lattice complex with characteristic Wyckoff position *Imma* 8*h* $0, y, z$ has the descriptive symbol .2. $B_b2yz$ for this position. Another Wyckoff position of this lattice complex is *Imma* 8*i* $x, \frac{1}{4}, z$. The corresponding point configurations are mapped onto each other by interchanging positive *x* and negative *y* directions and shifting by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. Therefore, the descriptive symbol for Wyckoff position *Imma i* is $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. $A_a2xz$.

In some cases, the Wyckoff position described by a lattice-complex symbol has more degrees of freedom than the lattice complex (see Section 3.4.1.5.1). In such cases, a letter (or a string of letters) in brackets is added to the symbol.

*Examples*

*tP*[*z*] for *P*4 *a*, *aP*[*xyz*] for *P*1 *a*.

#### 3.4.3.1.4. Properties of the descriptive symbols

Different kinds of relations between lattice complexes are brought out.

*Examples*

$P \leftrightarrow P4x \leftrightarrow P4x2z$, $\quad I4xxx \leftrightarrow ..2\ I4xxx$, $\quad P4x \leftrightarrow I4x$.

In many cases, limiting-complex relations can be deduced from the symbols. This applies to limiting complexes due either to special metrical parameters (*e.g.* $cP \leftrightarrow rP$ *etc.*) or to special values of coordinates (*e.g.* both *P*4*x* and *P*4*xx* are limiting complexes of *P*4*xy*). If the site set consists of only one point, the central part of the symbol specifies all corresponding limiting complexes without degrees of freedom that are due to special values of the coordinates (*e.g.* $2_12_1$. $FA_aB_bC_cI_aI_bI_c1xyz$ for the general position of $P2_12_12_1$).

### 3.4.3.2. Assignment of Wyckoff positions to Wyckoff sets and to lattice complexes

In Tables 3.4.3.2 and 3.4.3.3, the Wyckoff positions of all plane and space groups, respectively, are listed. Each Wyckoff position is identified by its Wyckoff letter together with its oriented site-symmetry symbol. It is assigned to its lattice complex by means of the reference symbol (*cf.* Section 3.4.1.3). Characteristic Wyckoff positions are marked by asterisks (*e.g.* 2*e* in $P2/c$). If in a particular space group several Wyckoff positions belong to the same Wyckoff set (*cf.* Sections 1.4.4.3 and 3.4.1.2; Koch & Fischer, 1975), the reference symbol is given only once (*e.g.* Wyckoff positions 4*l* to 4*o* in $P4/mmm$). To enable this, the usual sequence of Wyckoff positions had to be changed in a few cases (*e.g.* in $P4_2/mcm$). For Wyckoff positions assigned to the same lattice complex but belonging to different Wyckoff sets, the reference symbol is repeated. In $I4/m$, for example, Wyckoff positions 4*c* and 4*d* are both assigned to the lattice complex $P4/mmm$ *a*. They do not belong, however, to the same Wyckoff set because the site-symmetry groups $2/m$.. of 4*c* and $\bar{4}$.. of 4*d* are different.

The last columns of Tables 3.4.3.2 and 3.4.3.3 show the descriptive lattice-complex symbol for each Wyckoff position.

## 3.4.4. Applications of the lattice-complex concept

### 3.4.4.1. Geometrical properties of point configurations

To study the geometrical properties of all point configurations in three-dimensional space, it is not necessary to consider all Wyckoff positions of the space groups or all 1128 types of Wyckoff set. Instead, one may restrict the investigations to the characteristic Wyckoff positions of the 402 lattice complexes. The results can then be transferred to all non-characteristic Wyckoff positions of the lattice complexes, as listed in Tables 3.4.3.2 and 3.4.3.3.

The determination of all types of sphere packings with cubic and tetragonal symmetry forms an example for this kind of procedure (Fischer, 1973, 1974, 1991*a*,*b*, 1993). The cubic lattice complex *I*4*xxx*, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ 8*c* .3*m*. $x, x, x$. Sphere packings with three-membered rings and nine contacts per sphere are formed if $x = 3/16$. The parameter region $3/16 < x < \frac{1}{4}$ corresponds to sphere packings with four-membered rings and six contacts per sphere (*cf.* Fischer, 1973). $Ag_3PO_4$ crystallizes with symmetry $P\bar{4}3n$ (Deschizeaux-Cheruy *et al.*, 1982) and the oxygen atoms occupy Wyckoff position 8*e* .3. $x, x, x$, which also belongs to lattice complex *I*4*xxx*. Comparison of the coordinate parameter $x = 0.1491$ for the oxygen atoms with the sphere-packing parameters listed for $I\bar{4}3m$ *c* shows directly that the oxygen arrangement in this crystal structure does not form a sphere packing.

Other examples for this approach are the derivation of crystal potentials (Naor, 1958), of coordinate restrictions in

(*continued on page* 823)



references