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 ($Pmma$ $2e$ $\frac{1}{4}, 0, z$), 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 $1z$ 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 ($Pmma$ $4k$ $\frac{1}{4}, y, z$), 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 $2y$ 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 $Imma$ $8h$ $0, y, z$ has the descriptive symbol .2. B_b2yz for this position. Another Wyckoff position of this lattice complex is $Imma$ $8i$ $x, \frac{1}{4}, z$. 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 $P4$ a, $aP[xyz]$ for $P1$ a.

3.4.3.1.4. *Properties of the descriptive symbols*

Different kinds of relations between lattice complexes are brought out.

Examples

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

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 $P4x$ and $P4xx$ are limiting complexes of $P4xy$). 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.* $2e$ 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 $4l$ to $4o$ 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 $4c$ and $4d$ 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 $4c$ and $\bar{4}$.. of $4d$ 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 $I4xxx$, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ $8c$ $.3m.$ 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 $8e$ .3. x, x, x, which also belongs to lattice complex $I4xxx$. 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)