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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 β-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 noncharacteristic 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 *C* is represented in its characteristic Wyckoff position *Cmmm a* by the coordinate triplets 000 and $\frac{1}{2}\frac{1}{2}0$. In *Ibam a*, it is described by $00\frac{1}{4}$, $\frac{1}{2}\frac{1}{2}\frac{1}{4}$ and, therefore, receives the descriptive symbol $00\frac{1}{4}\ C$.

(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 000. It occurs also in *Pmma a* with coordinate triplets 000, $\frac{1}{2}00$, and in *Pcca a* with 000, $00\frac{1}{2}$, $\frac{1}{2}00$, $\frac{1}{2}0\frac{1}{2}$. 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 considered Wyckoff position is mapped onto the characteristic position by an inversion through the origin, *i.e.* both 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 000, $\frac{2}{3}\frac{1}{3}\frac{1}{3}$, $\frac{1}{3}\frac{2}{3}\frac{2}{3}$. The same lattice complex is symbolized by ${}'R_c$ in the noncharacteristic position $R\bar{3}c\ b$ with coordinate description 000, $00\frac{1}{2}$, $\frac{2}{3}\frac{1}{3}\frac{1}{3}$, $\frac{2}{3}\frac{1}{3}\frac{5}{6}$, $\frac{1}{3}\frac{2}{3}\frac{2}{3}$, $\frac{1}{3}\frac{2}{3}\frac{1}{6}$.

In noncharacteristic Wyckoff positions, the descriptive symbol *P* may be replaced by *C*, *I* by *F* (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).

14.2.3.3. *Lattice complexes with degrees of freedom*

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

Example

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

Normally, the central part is the symbol of an invariant lattice complex. Shift vector and central part together should be interpreted as described in Section 14.2.3.2. The point configurations of the regarded Wyckoff position 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 symmetrically 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) *I*4*xxx* ($I\bar{4}3m$ 8*c* *xxx*) designates a lattice complex, the point configurations of which are composed of tetrahedra 4*xxx* in parallel orientations replacing the points of a cubic body-centred lattice *I*. The vertices of these tetrahedra are located on body diagonals.

(2) ..2 *I*4*xxx* ($Pn\bar{3}m$ 8*e* *xxx*) represents the lattice complex for which, in contrast to the first example, the tetrahedra 4*xxx* around 000 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 $P4_2/mcm\ 8l\ x0\frac{1}{4}$. Each corresponding point configuration consists of squares of points 4*x* replacing the points of a tetragonal primitive lattice *P*. In comparison with *P*4*x*, $00\frac{1}{4}\ P_c4x$ shows a unit-cell enlargement by $\mathbf{c}' = 2\mathbf{c}$ and a subsequent shift by the vector $(00\frac{1}{4})$.

In the case of a Weissenberg complex, 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 regarded Weissenberg complex. 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* $\frac{1}{4}0z$), each of the two points $\frac{1}{4}00$ and $\frac{3}{4}00$, represented by $\frac{1}{4}00\ P_a$, is replaced by a site set containing only one point $1z$, *i.e.* the points 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 ($Pmma$ $4k$ $\frac{1}{4}yz$), each of the two points $\frac{1}{4}0z$ 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 dumb-bell. These dumb-bells are oriented parallel to the y axis.

The symbol of a noncharacteristic 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 $Imma$ $8h$ $0yz$ 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 14.2.2.1). In such a case, 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.

14.2.3.4. *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 $P4x$ 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 $P2_12_12_1$).

references