

14. LATTICE COMPLEXES

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 $\frac{1}{4}00 .2. P_a B 1 z 2 y$ ($Pmma 4k \frac{1}{4}yz$), each of the two points $\frac{1}{4}0z$ and $\frac{3}{4}0\bar{z}$, represented by $\frac{1}{4}00 .2. P_a B 1 z$, 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 $.2. B_b 2yz$ 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 $\frac{1}{4}\frac{1}{4}\frac{1}{4} .2.. A_a 2xz$.

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

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

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.* $2_1 2_1. FA_a B_b C_c I_a I_b I_c 1xyz$ for the general position of $P2_1 2_1 2_1$).