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Table 14.2.3.2. *Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes* (*cont.*)

96	*g*	..*m*	*	$Fd\bar{3}m$ *g*	..2 *D*6*z*2*xx*
96	*h*	..2	*	$Fd\bar{3}m$ *h*	$\bar{4}$.. *T*6$x\bar{x}$
192	*i*	1	*	$Fd\bar{3}m$ *i*	..2 *D*6*z*2*xx*2*y*
228	**$Fd\bar{3}c$**				
16	*a*	23.		$Im\bar{3}m$ *a*	I_2
32	*b*	.32		$Fm\bar{3}m$ *a*	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$ F_2
32	*c*	.$\bar{3}$.		$Fm\bar{3}m$ *a*	$\frac{3}{8}\frac{3}{8}\frac{3}{8}$ F_2
48	*d*	$\bar{4}$..		$Im\bar{3}m$ *b*	$J^*{}_2$
64	*e*	.3.		$Pn\bar{3}m$ *e*	(..2 *I*4*xxx*)$_2$
96	*f*	2..		$Im\bar{3}m$ *e*	$I_2$6*z*
96	*g*	..2	*	$Fd\bar{3}c$ *g*	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$ $\bar{4}$2.. $F_2$3$x\bar{x}$
192	*h*	1	*	$Fd\bar{3}c$ *h*	*d*.2 $I_2$6*z*2*xy*
229	**$Im\bar{3}m$**				
2	*a*	$m\bar{3}m$	*	$Im\bar{3}m$ *a*	*I*
6	*b*	4/*mm*.*m*	*	$Im\bar{3}m$ *b*	J^*
8	*c*	.$\bar{3}$*m*		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	$\bar{4}$*m*.2	*	$Im\bar{3}m$ *d*	W^*
12	*e*	4*m*.*m*	*	$Im\bar{3}m$ *e*	*I*6*z*
16	*f*	.3*m*	*	$Im\bar{3}m$ *f*	*I*8*xxx*
24	*g*	*mm*2..	*	$Im\bar{3}m$ *g*	.3. J^*4*x*
24	*h*	*m*.*m*2	*	$Im\bar{3}m$ *h*	*I*12*xx*
48	*i*	..2	*	$Im\bar{3}m$ *i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 4.. $P_2$6$x\bar{x}$
48	*j*	*m*..	*	$Im\bar{3}m$ *j*	*I*6*z*4*x*
48	*k*	..*m*	*	$Im\bar{3}m$ *k*	*I*6*z*4*xx*
96	*l*	1	*	$Im\bar{3}m$ *l*	*I*6*z*4*x*2*y*
230	**$Ia\bar{3}d$**				
16	*a*	.$\bar{3}$.		$Im\bar{3}m$ *a*	I_2
16	*b*	.32	*	$Ia\bar{3}d$ *b*	Y^{**}
24	*c*	2.22	*	$Ia\bar{3}d$ *c*	V^*
24	*d*	$\bar{4}$..	*	$Ia\bar{3}d$ *d*	S^*
32	*e*	.3.	*	$Ia\bar{3}d$ *e*	$\bar{4}$.. Y^{**}2*xxx*
48	*f*	2..	*	$Ia\bar{3}d$ *f*	.3. S^*2*z*
48	*g*	..2	*	$Ia\bar{3}d$ *g*	$\bar{4}$*a*.. Y^{**}3$x\bar{x}$
96	*h*	1	*	$Ia\bar{3}d$ *h*	$\bar{4}$*a*.. $I_2$6*xyz*

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 14.2.3.1 and 14.2.3.2 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.* The comparatively short descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

Table 14.2.3.3. *Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position*

Descriptive symbol	Crystal family	Characteristic Wyckoff position
C	*o* *m*	*Cmmm a* *C*2/*m a*
D	*c* *o*	$Fd\bar{3}m$ *a* *Fddd a*
^{v}D	*t*	$I4_1/amd$ *a*
E	*h*	$P6_3/mmc$ *c*
F	*c* *o*	$Fm\bar{3}m$ *a* *Fmmm a*
G	*h*	*P*6/*mmm c*
I	*c* *t* *o*	$Im\bar{3}m$ *a* *I*4/*mmm a* *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*	*P*6/*mmm f*
P	*c* *h* *t* *o* *m* *a*	$Pm\bar{3}m$ *a* *P*6/*mmm a* *P*4/*mmm a* *Pmmm a* *P*2/*m 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* *o*	$Fd\bar{3}m$ *c* *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*

14.2.3.2. *Invariant lattice complexes*

Invariant lattice complexes in their characteristic Wyckoff position are represented by a capital letter eventually in combination with some superscript. The first column of Table 14.2.3.3 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).

* Some of the descriptive symbols listed in Table 14.2.3.2 differ slightly from those derived by Fischer *et al.* (1973) and used in previous editions of *International Tables for Crystallography* Vol. A.

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

references