International Tables for Crystallography (2006). Vol. A, Chapter 14.2, pp. 848–872.

14.2. Symbols and properties of lattice complexes

By W. Fischer and E. Koch

14.2.1. Reference symbols and characteristic Wyckoff positions

If a lattice complex can be generated in different space-group types, one of them stands out because its corresponding Wyckoff positions show the highest site symmetry. This is called the *characteristic space-group type* of the lattice complex. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of the characteristic type.

Different lattice complexes may have the same characteristic space-group type but in that case they differ in the oriented site symmetry of their Wyckoff positions within the space groups of that type.

The characteristic space-group type and the corresponding oriented site symmetry express the common symmetry properties of all point configurations of a lattice complex. Therefore, they can be used to identify each lattice complex. Within the *reference symbols* of lattice complexes, however, instead of the site symmetry the Wyckoff letter of one of the Wyckoff positions with that site symmetry is given, as was first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Examples

(1) $Pm\bar{3}m$ is the characteristic space-group type for the lattice complex of all cubic primitive point lattices. The Wyckoff positions with the highest possible site symmetry $m\bar{3}m$ are 1*a* 000 and 1*b* $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, from which 1*a* has been chosen as the characteristic position. Thus, the lattice complex is designated $Pm\bar{3}m$ *a*.

(2) $Pm\bar{3}m$ is also characteristic for another lattice complex that corresponds to Wyckoff position 8*g* *xxx* $.3m$. Thus, the reference symbol for this lattice complex is $Pm\bar{3}m$ *g*. Each of its point configurations may be derived by replacing each point of a cubic primitive lattice by eight points arranged at the corners of a cube.

In Tables 14.2.3.1 and 14.2.3.2, the reference symbols denote the lattice complex of each Wyckoff position. The reference symbols of 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.* 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.

14.2.2. Additional properties of lattice complexes

14.2.2.1. *The degrees of freedom*

The number of coordinate parameters that can be varied independently within a Wyckoff position is called its number of degrees of freedom. For most lattice complexes, the number of *degrees of freedom* is the same as for any of its Wyckoff positions. The lattice complex with characteristic Wyckoff position $Pm\bar{3}$ 12*j* *m*.. 0*yz*, for instance, has two degrees of freedom. If, however, the variation of a coordinate corresponds to a shift of the point configuration as a whole, one degree of freedom is lost. Therefore, $I4_1$ 8*b* *xyz* is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8*b* itself has three degrees of freedom. Another example is given by $P4/m$ 4*j* *m*.. *xy*0 and *P*4 4*d* 1 *xyz*. Both Wyckoff positions belong to lattice complex $P4/m$ *j* with two degrees of freedom.

According to its number of degrees of freedom, a lattice complex is called *invariant, univariant, bivariant or trivariant.* In total, there exist 402 lattice complexes, 36 of which are invariant, 106 univariant, 105 bivariant and 155 trivariant. The 30 plane lattice complexes are made up of 7 invariant, 10 univariant and 13 bivariant ones.

Most of the invariant and univariant lattice complexes correspond to several types of Wyckoff set. In contrast to that, only one type of Wyckoff set belongs to each trivariant lattice complex. A bivariant lattice complex may either correspond to one type of Wyckoff set (*e.g.* $Pm\bar{3}$ *j*) or to two types (*P*4 *d*, for example, belongs to the lattice complex with the characteristic position $P4/m$ *j*).

14.2.2.2. *Limiting complexes and comprehensive complexes*

For point groups, the occurrence of limiting crystal forms is well known. In $4/m$, for instance, any tetragonal prism $\{hk0\}$ is a special crystal form with face symmetry *m*.. . In point group 4, on the other hand, the tetragonal prisms $\{hk0\}$ belong, as special cases, to the set of general crystal forms $\{hkl\}$, the tetragonal pyramids, and there is no difference between $\{hkl\}$ and $\{hk0\}$ in either the number or the symmetry of their faces. Therefore, the tetragonal prism is called a 'limiting form' of the tetragonal pyramid. In a case like this, all possible sets of equivalent faces belonging to a special type of crystal form (the tetragonal prism) may also be generated as a subset of another more comprehensive type of crystal form (the tetragonal pyramid). Of course, it is not possible, by considering a tetragonal prism by itself, to decide whether it has been generated by point group $4/m$ or by point group 4. This distinction can be made, however, if the tetragonal prism shows the right striations or occurs in combination with other appropriate crystal forms. Low quartz (oriented point group 321) gives a well known example: the hexagonal prism $\{10\bar{1}0\}$ has the same site symmetry 1 as any trigonal trapezohedron $\{hkil\}$. Therefore, $\{10\bar{1}0\}$ may be recognized as a limiting form only if the crystal shows in addition at least one trigonal trapezohedron.

A similar relation may exist between two lattice complexes. Let *L* be a lattice complex generated by a Wyckoff position of a space group $\mathcal{G}$ (*e.g.* by $P4/mmm$ 4*l* *m*2*m*. *x*00). An appropriate Wyckoff position of a subgroup $\mathcal{H}$ of $\mathcal{G}$ (*e.g.* $P4/m$ 4*j* *m*.. *xy*0) may produce not only all point configurations of *L* but other point configurations in addition (with different orientations of the squares in the example). The complete set then forms a second lattice complex *M*. Such relationships led to the following definition (Fischer & Koch, 1974, 1978):

> If a lattice complex *L* forms a true subset of another lattice complex *M*, the lattice complex *L* is called a *limiting complex* of *M* and the lattice complex *M* a *comprehensive complex* of *L.*

The point configurations of the limiting complex *L* are generated within *M* by restrictions imposed on the coordinate or/and the metrical parameters.

In the above example, such a restriction holds for the *y* coordinate: the condition $y = 0$ for Wyckoff position 4*j* of $P4/m$ filters out exactly those point configurations that constitute the lattice complex $P4/mmm\ l$. The latter complex is, therefore, a limiting complex of the lattice complex $P4/m\ j$. In the present case of restricted coordinates, both complexes belong to the same crystal family and L has fewer degrees of freedom than M.

Another kind of limiting-complex relation is connected with restrictions for metrical parameters. All point configurations of the lattice complex $Pm\bar{3}m\ a$ are also generated by $P4/mmm\ a$ under the restriction $a = c$, *i.e.* in special space groups of type $P4/mmm$. Here L and M have the same number of degrees of freedom, but belong to different crystal families.

Finally, the two types of parameter restrictions for limiting complexes may also occur in combination. The trivariant lattice complex with characteristic Wyckoff position $P4_12_12\ 8b\ xyz$, for example, contains the invariant cubic lattice complex $Fm\bar{3}m\ a$ as a limiting complex. The parameter restrictions necessary are $x = \frac{1}{2}, y = 0, z = \frac{1}{16}, c/a = 4\sqrt{2}$.

As for a limiting form in crystal morphology, it is often impossible to decide by which symmetry (space group and Wyckoff set) a particular point configuration, regarded by itself, has been generated. If a point configuration belongs to a lattice complex that is part of a comprehensive complex, this point configuration is a member of both complexes. As a consequence, the lattice complexes do not form equivalence classes of point configurations. Only if a point configuration is inspected in combination with a sufficient number of other point configurations – like sets of symmetrically equivalent atoms in a crystal structure – does it make sense to assign this point configuration to a particular lattice complex. An example is found in the crystal structures of the spinel type. Here, the oxygen atoms occupy Wyckoff position $32e\ xxx$ in $Fd\bar{3}m$ with $x \approx \frac{3}{8}$ (referred to origin choice 1). If x is restricted to $\frac{3}{8}$, the point configurations generated are those of the lattice complex $Fm\bar{3}m\ a$ (formed by all face-centred cubic point lattices). If for a spinel-type structure this restriction holds exactly, the point configurations of the cations would, nevertheless, reveal the true generating symmetry of the oxygen point configuration. It has, therefore, to be considered a member of the comprehensive complex $Fd\bar{3}m\ e$ rather than a member of the lattice complex $Fm\bar{3}m\ a$ (which includes among others the point configuration of the copper atoms in the crystal structure of copper). For practical applications, a point configuration contained in several lattice complexes may be investigated within the complex that is the least comprehensive but still allows the physical behaviour under discussion. This corresponds to the definition of the symmetry of a crystal generally used in crystallography: the highest symmetry that can be assigned to a crystal as a whole is that of its least symmetrical property known to date.

Even though limiting-complex relations are very useful for establishing crystallochemical relationships between different crystal structures, a complete study has not yet been carried out. Apart from isolated examples in the literature, systematic treatments have been given only for special aspects: plane lattice complexes (Burzlaff *et al.*, 1968); cubic lattice complexes (Koch, 1974); point complexes, rod complexes and layer complexes (Fischer & Koch, 1978); extraordinary orbits for plane groups (Lawrenson & Wondratschek, 1976); noncharacteristic orbits of space groups except those that are due to metrical specialization (Engel *et al.*, 1984). The closely related concepts of limiting complexes and noncharacteristic orbits have been compared by Koch & Fischer (1985).

14.2.2.3. *Weissenberg complexes*

Depending on their site-symmetry groups, two kinds of Wyckoff position may be distinguished:

(i) The site-symmetry group of any point is a proper subgroup of another site-symmetry group from the same space group. Then, the Wyckoff position contains, among others, point configurations with the property that the distance between two suitable chosen points is shorter than any small number $\varepsilon > 0$.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm\ 4j\ m.2m\ xx0$ may be imagined as squares of four points surrounding the points of a tetragonal primitive lattice. For $x \to 0$, the squares become infinitesimally small. Point configurations with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to lattice complex $P4/mmm\ a$.

(ii) The site-symmetry group of any point belonging to the regarded Wyckoff position is not a subgroup of any other site-symmetry group from the same space group.

Example

In $Pmma$, there does not exist a site-symmetry group that is a proper supergroup of $mm2$, the site-symmetry group of Wyckoff position $Pmma\ 2e\ \frac{1}{4}0z$. As a consequence, the distance between any two symmetrically equivalent points belonging to $Pmma\ e$ cannot become shorter than the minimum of $\frac{1}{2}a, b$ and c.

A lattice complex contains either Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are made up from Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes that do not contain point configurations with infinitesimal short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes have been called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. In addition, there exist 24 univariant (monoclinic 2, orthorhombic 5, tetragonal 7, hexagonal 5, cubic 5) and 6 bivariant Weissenberg complexes (monoclinic 1, orthorhombic 2, tetragonal 1, hexagonal 2). The only trivariant Weissenberg complex is $P2_12_12_1\ a$. All Weissenberg complexes with degrees of freedom have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family.

Example

$Pmma\ e$ is a comprehensive complex of $Pmmm\ a$ and of $Cmmm\ a$. Within the characteristic Wyckoff position, $\frac{1}{4}00$ refers to $Pmmm\ a$ and $\frac{1}{4}0\frac{1}{4}$ to $Cmmm\ a$.

Except for the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex $p2mg\ c$.

14.2.3. Descriptive symbols

14.2.3.1. *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

(*continued on page* 870)

Table 14.2.3.1. *Plane groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes*

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1 *p*1

1	*a*	1	*p*2 *a*	*P*[*xy*]

2 *p*2

1	*a*	2	* *p*2 *a*	*P*
1	*b*			$0\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	1	* *p*2 *e*	*P*2*xy*

3 *pm*

1	*a*	.*m*.	*p*2*mm a*	*P*[*y*]
1	*b*			$\frac{1}{2}0$ *P*[*y*]
2	*c*	1	*p*2*mm e*	*P*2*x*[*y*]

4 *pg*

2	*a*	1	*p*2*mg c*	2.. $P_bC1x[y]$

5 *cm*

2	*a*	.*m*.	*c*2*mm a*	*C*[*y*]
4	*b*	1	*c*2*mm d*	*C*2*x*[*y*]

6 *p*2*mm*

1	*a*	2*mm*	* *p*2*mm a*	*P*
1	*b*			$0\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	..*m*	* *p*2*mm e*	*P*2*x*
2	*f*			$0\frac{1}{2}$ *P*2*x*
2	*g*	.*m*.		*P*2*y*
2	*h*			$\frac{1}{2}0$ *P*2*y*
4	*i*	1	* *p*2*mm i*	*P*2*x*2*y*

7 *p*2*mg*

2	*a*	2..	*p*2*mm a*	P_a
2	*b*			$0\frac{1}{2}$ P_a
2	*c*	.*m*.	* *p*2*mg c*	$\frac{1}{4}0$ 2.. P_aC1y
4	*d*	1	* *p*2*mg d*	.*m*. P_a2xy

8 *p*2*gg*

2	*a*	2..	*c*2*mm a*	*C*
2	*b*			$\frac{1}{2}0$ *C*
4	*c*	1	* *p*2*gg c*	.*g*. *C*2*xy*

9 *c*2*mm*

2	*a*	2*mm*	* *c*2*mm a*	*C*
2	*b*			$0\frac{1}{2}$ *C*
4	*c*	2..	*p*2*mm a*	$\frac{1}{4}\frac{1}{4}$ P_{ab}
4	*d*	..*m*	* *c*2*mm d*	*C*2*x*
4	*e*	.*m*.		*C*2*y*
8	*f*	1	* *c*2*mm f*	*C*2*x*2*y*

10 *p*4

1	*a*	4..	*p*4*mm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}$ *P*
2	*c*	2..	*p*4*mm a*	$0\frac{1}{2}$ *C*
4	*d*	1	* *p*4 *d*	*P*4*xy*

11 *p*4*mm*

1	*a*	4*mm*	* *p*4*mm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}$ *P*
2	*c*	2*mm*.	*p*4*mm a*	$0\frac{1}{2}$ *C*
4	*d*	.*m*.	* *p*4*mm d*	*P*4*x*
4	*e*			$\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*f*	..*m*	* *p*4*mm f*	*P*4*xx*
8	*g*	1	* *p*4*mm g*	*P*4*x*2*y*

12 *p*4*gm*

2	*a*	4..	*p*4*mm a*	*C*
2	*b*	2.*mm*	*p*4*mm a*	$0\frac{1}{2}$ *C*
4	*c*	..*m*	* *p*4*gm c*	$0\frac{1}{2}$.*g*. *C*2*xx*
8	*d*	1	* *p*4*gm d*	..*m* *C*4*xy*

13 *p*3

1	*a*	3..	*p*6*mm a*	*P*
1	*b*			$\frac{1}{3}\frac{2}{3}$ *P*
1	*c*			$\frac{2}{3}\frac{1}{3}$ *P*
3	*d*	1	* *p*3 *d*	*P*3*xy*

14 *p*3*m*1

1	*a*	3*m*.	*p*6*mm a*	*P*
1	*b*			$\frac{1}{3}\frac{2}{3}$ *P*
1	*c*			$\frac{2}{3}\frac{1}{3}$ *P*
3	*d*	.*m*.	* *p*3*m*1 *d*	$P3x\bar{x}$
6	*e*	1	* *p*3*m*1 *e*	$P3x\bar{x}2y$

15 *p*31*m*

1	*a*	3.*m*	*p*6*mm a*	*P*
2	*b*	3..	*p*6*mm b*	*G*
3	*c*	..*m*	* *p*31*m c*	*P*3*x*
6	*d*	1	* *p*31*m d*	*P*3*x*2*y*

16 *p*6

1	*a*	6..	*p*6*mm a*	*P*
2	*b*	3..	*p*6*mm b*	*G*
3	*c*	2..	*p*6*mm c*	*N*
6	*d*	1	* *p*6 *d*	*P*6*xy*

17 *p*6*mm*

1	*a*	6*mm*	* *p*6*mm a*	*P*
2	*b*	3*m*.	* *p*6*mm b*	*G*
3	*c*	2*mm*	* *p*6*mm c*	*N*
6	*d*	..*m*	* *p*6*mm d*	*P*6*x*
6	*e*	.*m*.	* *p*6*mm e*	$P6x\bar{x}$
12	*f*	1	* *p*6*mm f*	*P*6*x*2*y*

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

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1	***P*1**		
1	*a* 1	$P\bar{1}$ *a*	*P*[*xyz*]
2	***P*$\bar{1}$**		
1	*a* $\bar{1}$	* $P\bar{1}$ *a*	*P*
1	*b*		$00\frac{1}{2}$ *P*
1	*c*		$0\frac{1}{2}0$ *P*
1	*d*		$\frac{1}{2}00$ *P*
1	*e*		$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*		$\frac{1}{2}0\frac{1}{2}$ *P*
1	*g*		$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*		$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*i* 1	* $P\bar{1}$ *i*	*P*2*xyz*
3	***P*2**		
1	*a* 2	*P*2/*m a*	*P*[*y*]
1	*b*		$00\frac{1}{2}$ *P*[*y*]
1	*c*		$\frac{1}{2}00$ *P*[*y*]
1	*d*		$\frac{1}{2}0\frac{1}{2}$ *P*[*y*]
2	*e* 1	*P*2/*m m*	*P*2*xz*[*y*]
4	***P*2$_1$**		
2	*a* 1	$P2_1/m$ *e*	2_1 $P_bACI1xz[y]$
5	***C*2**		
2	*a* 2	*C*2/*m a*	*C*[*y*]
2	*b*		$00\frac{1}{2}$ *C*[*y*]
4	*c* 1	*C*2/*m i*	*C*2*xz*[*y*]
6	***Pm***		
1	*a m*	*P*2/*m a*	*P*[*xz*]
1	*b*		$0\frac{1}{2}0$ *P*[*xz*]
2	*c* 1	*P*2/*m i*	*P*2*y*[*xz*]
7	***Pc***		
2	*a* 1	*P*2/*c e*	*c* $P_cA1y[xz]$
8	***Cm***		
2	*a m*	*C*2/*m a*	*C*[*xz*]
4	*b* 1	*C*2/*m g*	*C*2*y*[*xz*]
9	***Cc***		
4	*a* 1	*C*2/*c e*	$\bar{1}$ $C_cF1y[xz]$
10	***P*2/*m***		
1	*a* 2/*m*	* *P*2/*m a*	*P*
1	*b*		$0\frac{1}{2}0$ *P*
1	*c*		$00\frac{1}{2}$ *P*
1	*d*		$\frac{1}{2}00$ *P*
1	*e*		$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*		$0\frac{1}{2}\frac{1}{2}$ *P*
1	*g*		$\frac{1}{2}0\frac{1}{2}$ *P*
1	*h*		$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*i* 2	* *P*2/*m i*	*P*2*y*
2	*j*		$\frac{1}{2}00$ *P*2*y*
2	*k*		$00\frac{1}{2}$ *P*2*y*
2	*l*		$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*m m*	* *P*2/*m m*	*P*2*xz*
2	*n*		$0\frac{1}{2}0$ *P*2*xz*
4	*o* 1	* *P*2/*m o*	*P*2*xz*2*y*
11	***P*2$_1$/*m***		
2	*a* $\bar{1}$	*P*2/*m a*	P_b
2	*b*		$\frac{1}{2}00$ P_b
2	*c*		$00\frac{1}{2}$ P_b
2	*d*		$\frac{1}{2}0\frac{1}{2}$ P_b
2	*e m*	* $P2_1/m$ *e*	$0\frac{1}{4}0$ $2_1P_bACI1xz$
4	*f* 1	* $P2_1/m$ *f*	*m* P_b2xyz
12	***C*2/*m***		
2	*a* 2/*m*	* *C*2/*m a*	*C*
2	*b*		$0\frac{1}{2}0$ *C*
2	*c*		$00\frac{1}{2}$ *C*
2	*d*		$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e* $\bar{1}$	*P*2/*m a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*		$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g* 2	* *C*2/*m g*	*C*2*y*
4	*h*		$00\frac{1}{2}$ *C*2*y*
4	*i m*	* *C*2/*m i*	*C*2*xz*
8	*j* 1	* *C*2/*m j*	*C*2*xz*2*y*
13	***P*2/*c***		
2	*a* $\bar{1}$	*P*2/*m a*	P_c
2	*b*		$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*		$0\frac{1}{2}0$ P_c
2	*d*		$\frac{1}{2}00$ P_c
2	*e* 2	* *P*2/*c e*	$00\frac{1}{4}$ *c* P_cA1y
2	*f*		$\frac{1}{2}0\frac{1}{4}$ *c* P_cA1y
4	*g* 1	* *P*2/*c g*	2 P_c2xyz
14	***P*2$_1$/*c***		
2	*a* $\bar{1}$	*C*2/*m a*	*A*
2	*b*		$\frac{1}{2}00$ *A*
2	*c*		$00\frac{1}{2}$ *A*
2	*d*		$\frac{1}{2}0\frac{1}{2}$ *A*
4	*e* 1	* $P2_1/c$ *e*	*c A*2*xyz*
15	***C*2/*c***		
4	*a* $\bar{1}$	*C*2/*m a*	C_c
4	*b*		$0\frac{1}{2}0$ C_c
4	*c*		$\frac{1}{4}\frac{1}{4}0$ *F*
4	*d*		$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ *F*
4	*e* 2	* *C*2/*c e*	$00\frac{1}{4}$ $\bar{1}$ C_cF1y
8	*f* 1	* *C*2/*c f*	2_1 C_c2xyz
16	***P*222**		
1	*a* 222	*Pmmm a*	*P*
1	*b*		$\frac{1}{2}00$ *P*
1	*c*		$0\frac{1}{2}0$ *P*
1	*d*		$00\frac{1}{2}$ *P*
1	*e*		$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*		$\frac{1}{2}0\frac{1}{2}$ *P*
1	*g*		$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*		$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*

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

2	*i*	2..	*Pmmm i*	*P*2*x*
2	*j*			$00\frac{1}{2}$ *P*2*x*
2	*k*			$0\frac{1}{2}0$ *P*2*x*
2	*l*			$0\frac{1}{2}\frac{1}{2}$ *P*2*x*
2	*m*	.2.		*P*2*y*
2	*n*			$00\frac{1}{2}$ *P*2*y*
2	*o*			$\frac{1}{2}00$ *P*2*y*
2	*p*			$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*q*	..2		*P*2*z*
2	*r*			$\frac{1}{2}00$ *P*2*z*
2	*s*			$0\frac{1}{2}0$ *P*2*z*
2	*t*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*u*	1	* *P*222 *u*	*P*2*x*2*yz*
17	$\boldsymbol{P222_1}$			
2	*a*	2..	*Pmma e*	.2. P_cB1x
2	*b*			$0\frac{1}{2}0$ .2. P_cB1x
2	*c*	.2.		$00\frac{1}{4}$ 2.. P_cA1y
2	*d*			$\frac{1}{2}0\frac{1}{4}$ 2.. P_cA1y
4	*e*	1	* $P222_1$ *e*	.2. $P_cB1x2yz$
18	$\boldsymbol{P2_12_12}$			
2	*a*	..2	*Pmmn a*	2_1.. *CI*1*z*
2	*b*			$0\frac{1}{2}0$ 2_1.. *CI*1*z*
4	*c*	1	* $P2_12_12$ *c*	2_1.. *CI*1*z*2*xy*
19	$\boldsymbol{P2_12_12_1}$			
4	*a*	1	* $P2_12_12_1$ *a*	2_12_1. $FA_aB_bC_cI_aI_bI_c1xyz$
20	$\boldsymbol{C222_1}$			
4	*a*	2..	*Cmcm c*	.2_1. C_cF1x
4	*b*	.2.		$00\frac{1}{4}$ 2_1.. C_cF1y
8	*c*	1	* $C222_1$ *c*	.2_1. $C_cF1x2yz$
21	***C*222**			
2	*a*	222	*Cmmm a*	*C*
2	*b*			$0\frac{1}{2}0$ *C*
2	*c*			$\frac{1}{2}0\frac{1}{2}$ *C*
2	*d*			$00\frac{1}{2}$ *C*
4	*e*	2..	*Cmmm g*	*C*2*x*
4	*f*			$00\frac{1}{2}$ *C*2*x*
4	*g*	.2.		*C*2*y*
4	*h*			$00\frac{1}{2}$ *C*2*y*
4	*i*	..2	*Cmmm k*	*C*2*z*
4	*j*			$0\frac{1}{2}0$ *C*2*z*
4	*k*	..2	*Cmme g*	$\frac{1}{4}\frac{1}{4}0$ 2.. $P_{ab}F1z$
8	*l*	1	* *C*222 *l*	*C*2*x*2*yz*
22	***F*222**			
4	*a*	222	*Fmmm a*	*F*
4	*b*			$00\frac{1}{2}$ *F*
4	*c*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
8	*e*	2..	*Fmmm g*	*F*2*x*
8	*j*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*x*
8	*f*	.2.		*F*2*y*
8	*i*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*y*
8	*g*	..2		*F*2*z*
8	*h*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*z*
16	*k*	1	* *F*222 *k*	*F*2*x*2*yz*
23	***I*222**			
2	*a*	222	*Immm a*	*I*
2	*b*			$\frac{1}{2}00$ *I*
2	*c*			$00\frac{1}{2}$ *I*
2	*d*			$0\frac{1}{2}0$ *I*
4	*e*	2..	*Immm e*	*I*2*x*
4	*f*			$00\frac{1}{2}$ *I*2*x*
4	*g*	.2.		*I*2*y*
4	*h*			$\frac{1}{2}00$ *I*2*y*
4	*i*	..2		*I*2*z*
4	*j*			$0\frac{1}{2}0$ *I*2*z*
8	*k*	1	* *I*222 *k*	*I*2*x*2*yz*
24	$\boldsymbol{I2_12_12_1}$			
4	*a*	2..	*Imma e*	$\frac{1}{4}0\frac{1}{4}$ ..2 C_cB_b1x
4	*b*	.2.		$\frac{1}{4}\frac{1}{4}0$ 2.. A_aC_c1y
4	*c*	..2		$0\frac{1}{4}\frac{1}{4}$ .2. B_bA_a1z
8	*d*	1	* $I2_12_12_1$ *d*	$\frac{1}{4}0\frac{1}{4}$ ..2 C_cB_b1x2yz
25	***Pmm*2**			
1	*a*	*mm*2	*Pmmm a*	*P*[*z*]
1	*b*			$0\frac{1}{2}0$ *P*[*z*]
1	*c*			$\frac{1}{2}00$ *P*[*z*]
1	*d*			$\frac{1}{2}\frac{1}{2}0$ *P*[*z*]
2	*e*	.*m*.	*Pmmm i*	*P*2*x*[*z*]
2	*f*			$0\frac{1}{2}0$ *P*2*x*[*z*]
2	*g*	*m*..		*P*2*y*[*z*]
2	*h*			$\frac{1}{2}00$ *P*2*y*[*z*]
4	*i*	1	*Pmmm u*	*P*2*x*2*y*[*z*]
26	$\boldsymbol{Pmc2_1}$			
2	*a*	*m*..	*Pmma e*	2.. $P_cA1y[z]$
2	*b*			$\frac{1}{2}00$ 2.. $P_cA1y[z]$
4	*c*	1	*Pmma k*	2.. $P_cA1y2x[z]$
27	***Pcc*2**			
2	*a*	..2	*Pmmm a*	$P_c[z]$
2	*b*			$0\frac{1}{2}0$ $P_c[z]$
2	*c*			$\frac{1}{2}00$ $P_c[z]$
2	*d*			$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
4	*e*	1	*Pccm q*	2.. $P_c2xy[z]$
28	***Pma*2**			
2	*a*	..2	*Pmmm a*	$P_a[z]$
2	*b*			$0\frac{1}{2}0$ $P_a[z]$
2	*c*	*m*..	*Pmma e*	$\frac{1}{4}00$ ..2 $P_aC1y[z]$
4	*d*	1	*Pmma i*	*m*.. $P_a2xy[z]$
29	$\boldsymbol{Pca2_1}$			
4	*a*	1	*Pbcm d*	.2$\bar{1}$ $P_{ac}B_aC_cF1xy[z]$
30	***Pnc*2**			
2	*a*	..2	*Cmmm a*	*A*[*z*]
2	*b*			$\frac{1}{2}00$ *A*[*z*]
4	*c*	1	*Pmna h*	2.. *A*2*xy*[*z*]

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

31	***Pmn*2$_1$**			
2	*a*	*m..*	*Pmmn a*	$..2_1$ *BI*1*y*[*z*]
4	*b*	1	*Pmmn e*	$..2_1$ *BI*1*y*2*x*[*z*]
32	***Pba*2**			
2	*a*	..2	*Cmmm a*	*C*[*z*]
2	*b*			$0\frac{1}{2}0$ *C*[*z*]
4	*c*	1	*Pbam g*	*b..* *C*2*xy*[*z*]
33	***Pna*2$_1$**			
4	*a*	1	*Pnma c*	$\bar{1}2_1.$ $C_cA_aFI_a$1*xy*[*z*]
34	***Pnn*2**			
2	*a*	..2	*Immm a*	*I*[*z*]
2	*b*			$0\frac{1}{2}0$ *I*[*z*]
4	*c*	1	*Pnnm g*	*n..* *I*2*xy*[*z*]
35	***Cmm*2**			
2	*a*	*mm*2	*Cmmm a*	*C*[*z*]
2	*b*			$0\frac{1}{2}0$ *C*[*z*]
4	*c*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}[*z*]
4	*d*	*.m.*	*Cmmm g*	*C*2*x*[*z*]
4	*e*	*m..*		*C*2*y*[*z*]
8	*f*	1	*Cmmm p*	*C*2*x*2*y*[*z*]
36	***Cmc*2$_1$**			
4	*a*	*m..*	*Cmcm c*	$2_1..$ C_cF1*y*[*z*]
8	*b*	1	*Cmcm g*	$2_1..$ C_cF1*y*2*x*[*z*]
37	***Ccc*2**			
4	*a*	..2	*Cmmm a*	C_c[*z*]
4	*b*			$0\frac{1}{2}0$ C_c[*z*]
4	*c*	..2	*Fmmm a*	$\frac{1}{4}\frac{1}{4}0$ *F*[*z*]
8	*d*	1	*Cccm l*	*n..* C_c2*xy*[*z*]
38	***Amm*2**			
2	*a*	*mm*2	*Cmmm a*	*A*[*z*]
2	*b*			$\frac{1}{2}00$ *A*[*z*]
4	*c*	*.m.*	*Cmmm k*	*A*2*x*[*z*]
4	*d*	*m..*	*Cmmm g*	*A*2*y*[*z*]
4	*e*			$\frac{1}{2}00$ *A*2*y*[*z*]
8	*f*	1	*Cmmm n*	*A*2*x*2*y*[*z*]
39	***Aem*2**			
4	*a*	..2	*Pmmm a*	P_{bc}[*z*]
4	*b*			$\frac{1}{2}00$ P_{bc}[*z*]
4	*c*	*.m.*	*Cmme g*	$0\frac{1}{4}0$ ..2 $P_{bc}F$1*x*[*z*]
8	*d*	1	*Cmme m*	*.m.* P_{bc}2*xy*[*z*]
40	***Ama*2**			
4	*a*	..2	*Cmmm a*	A_a[*z*]
4	*b*	*m..*	*Cmcm c*	$\frac{1}{4}00$ $..2_1$ A_aF1*y*[*z*]
8	*c*	1	*Cmcm f*	*.n.* A_a2*xy*[*z*]
41	***Aea*2**			
4	*a*	..2	*Fmmm a*	*F*[*z*]
8	*b*	1	*Cmce f*	*.2.* *F*2*xy*[*z*]

42	***Fmm*2**			
4	*a*	*mm*2	*Fmmm a*	*F*[*z*]
8	*b*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2[*z*]
8	*c*	*m..*	*Fmmm g*	*F*2*y*[*z*]
8	*d*	*.m.*		*F*2*x*[*z*]
16	*e*	1	*Fmmm m*	*F*2*x*2*y*[*z*]
43	***Fdd*2**			
8	*a*	..2	*Fddd a*	*D*[*z*]
16	*b*	1	* *Fdd*2 *b*	*d..* *D*2*xy*[*z*]
44	***Imm*2**			
2	*a*	*mm*2	*Immm a*	*I*[*z*]
2	*b*			$0\frac{1}{2}0$ *I*[*z*]
4	*c*	*.m.*	*Immm e*	*I*2*x*[*z*]
4	*d*	*m..*		*I*2*y*[*z*]
8	*e*	1	*Immm l*	*I*2*x*2*y*[*z*]
45	***Iba*2**			
4	*a*	..2	*Cmmm a*	C_c[*z*]
4	*b*			$0\frac{1}{2}0$ C_c[*z*]
8	*c*	1	*Ibam j*	*b..* C_c2*xy*[*z*]
46	***Ima*2**			
4	*a*	..2	*Cmmm a*	A_a[*z*]
4	*b*	*m..*	*Imma e*	$\frac{1}{4}00$ 2.. A_aC_c1*y*[*z*]
8	*c*	1	*Imma h*	2.. A_a2*xy*[*z*]
47	***Pmmm***			
1	*a*	*mmm*	* *Pmmm a*	*P*
1	*b*			$\frac{1}{2}00$ *P*
1	*c*			$00\frac{1}{2}$ *P*
1	*d*			$\frac{1}{2}0\frac{1}{2}$ *P*
1	*e*			$0\frac{1}{2}0$ *P*
1	*f*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*g*			$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
2	*i*	2*mm*	* *Pmmm i*	*P*2*x*
2	*j*			$00\frac{1}{2}$ *P*2*x*
2	*k*			$0\frac{1}{2}0$ *P*2*x*
2	*l*			$0\frac{1}{2}\frac{1}{2}$ *P*2*x*
2	*m*	*m*2*m*		*P*2*y*
2	*n*			$00\frac{1}{2}$ *P*2*y*
2	*o*			$\frac{1}{2}00$ *P*2*y*
2	*p*			$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*q*	*mm*2		*P*2*z*
2	*r*			$0\frac{1}{2}0$ *P*2*z*
2	*s*			$\frac{1}{2}00$ *P*2*z*
2	*t*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*u*	*m..*	* *Pmmm u*	*P*2*y*2*z*
4	*v*			$\frac{1}{2}00$ *P*2*y*2*z*
4	*w*	*.m.*		*P*2*x*2*z*
4	*x*			$0\frac{1}{2}0$ *P*2*x*2*z*
4	*y*	*..m*		*P*2*x*2*y*
4	*z*			$00\frac{1}{2}$ *P*2*x*2*y*
8	α	1	* *Pmmm* α	*P*2*x*2*y*2*z*

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

48 *Pnnn*

2	*a*	222	*Immm a*	I
2	*b*			$\frac{1}{2}00\ I$
2	*c*			$00\frac{1}{2}\ I$
2	*d*			$0\frac{1}{2}0\ I$
4	*e*	$\bar{1}$	*Fmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*f*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
4	*g*	2..	*Immm e*	$I2x$
4	*h*			$00\frac{1}{2}\ I2x$
4	*i*	.2.		$I2y$
4	*j*			$\frac{1}{2}00\ I2y$
4	*k*	..2		$I2z$
4	*l*			$0\frac{1}{2}0\ I2z$
8	*m*	1	* *Pnnn m*	$n..\ I2x2yz$

49 *Pccm*

2	*a*	..2/*m*	*Pmmm a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0\ P_c$
2	*c*			$0\frac{1}{2}0\ P_c$
2	*d*			$\frac{1}{2}00\ P_c$
2	*e*	222	*Pmmm a*	$00\frac{1}{4}\ P_c$
2	*f*			$\frac{1}{2}0\frac{1}{4}\ P_c$
2	*g*			$0\frac{1}{2}\frac{1}{4}\ P_c$
2	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ P_c$
4	*i*	2..	*Pmmm i*	$00\frac{1}{4}\ P_c2x$
4	*j*			$0\frac{1}{2}\frac{1}{4}\ P_c2x$
4	*k*	.2.		$00\frac{1}{4}\ P_c2y$
4	*l*			$\frac{1}{2}0\frac{1}{4}\ P_c2y$
4	*m*	..2	*Pmmm i*	P_c2z
4	*n*			$\frac{1}{2}\frac{1}{2}0\ P_c2z$
4	*o*			$0\frac{1}{2}0\ P_c2z$
4	*p*			$\frac{1}{2}00\ P_c2z$
4	*q*	..*m*	* *Pccm q*	$2..\ P_c2xy$
8	*r*	1	* *Pccm r*	$c..\ P_c2xy2z$

50 *Pban*

2	*a*	222	*Cmmm a*	C
2	*b*			$\frac{1}{2}00\ C$
2	*c*			$\frac{1}{2}0\frac{1}{2}\ C$
2	*d*			$00\frac{1}{2}\ C$
4	*e*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	2..	*Cmmm g*	$C2x$
4	*h*			$00\frac{1}{2}\ C2x$
4	*i*	.2.		$C2y$
4	*j*			$00\frac{1}{2}\ C2y$
4	*k*	..2	*Cmmm k*	$C2z$
4	*l*			$0\frac{1}{2}0\ C2z$
8	*m*	1	* *Pban m*	$b..\ C2x2yz$

51 *Pmma*

2	*a*	.2/*m*.	*Pmmm a*	P_a
2	*b*			$0\frac{1}{2}0\ P_a$
2	*c*			$00\frac{1}{2}\ P_a$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ P_a$
2	*e*	*mm*2	* *Pmma e*	$\frac{1}{4}00\ .2.\ P_aB1z$
2	*f*			$\frac{1}{4}\frac{1}{2}0\ .2.\ P_aB1z$
4	*g*	.2.	*Pmmm i*	P_a2y
4	*h*			$00\frac{1}{2}\ P_a2y$
4	*i*	.*m*.	* *Pmma i*	$m..\ P_a2xz$
4	*j*			$0\frac{1}{2}0\ m..\ P_a2xz$
4	*k*	*m*..	* *Pmma k*	$\frac{1}{4}00\ .2.\ P_aB1z2y$
8	*l*	1	* *Pmma l*	$m..\ P_a2xz2y$

52 *Pnna*

4	*a*	$\bar{1}$	*Cmmm a*	A_a
4	*b*			$00\frac{1}{2}\ A_a$
4	*c*	..2	*Imma e*	$\frac{1}{4}0\frac{1}{4}\ .2.\ B_bA_a1z$
4	*d*	2..	*Cmcm c*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ ..2_1\ B_bF1x$
8	*e*	1	* *Pnna e*	$2.2\ A_a2xyz$

53 *Pmna*

2	*a*	2/*m*..	*Cmmm a*	B
2	*b*			$\frac{1}{2}00\ B$
2	*c*			$\frac{1}{2}\frac{1}{2}0\ B$
2	*d*			$0\frac{1}{2}0\ B$
4	*e*	2..	*Cmmm g*	$B2x$
4	*f*			$0\frac{1}{2}0\ B2x$
4	*g*	.2.	*Pmma e*	$\frac{1}{4}0\frac{1}{4}\ (2..\ P_cA1y)_a$
4	*h*	*m*..	* *Pmna h*	$.2.\ B2yz$
8	*i*	1	* *Pmna i*	$.2.\ B2yz2x$

54 *Pcca*

4	*a*	$\bar{1}$	*Pmmm a*	P_{ac}
4	*b*			$0\frac{1}{2}0\ P_{ac}$
4	*c*	.2.	*Cmme g*	$00\frac{1}{4}\ ..2\ P_{ac}F1y$
4	*d*	..2	*Pmma e*	$\frac{1}{4}00\ (.2.\ P_aB1z)_c$
4	*e*			$\frac{1}{4}\frac{1}{2}0\ (.2.\ P_aB1z)_c$
8	*f*	1	* *Pcca f*	$.22\ P_{ac}2xyz$

55 *Pbam*

2	*a*	..2/*m*	*Cmmm a*	C
2	*b*			$00\frac{1}{2}\ C$
2	*c*			$0\frac{1}{2}0\ C$
2	*d*			$0\frac{1}{2}\frac{1}{2}\ C$
4	*e*	..2	*Cmmm k*	$C2z$
4	*f*			$0\frac{1}{2}0\ C2z$
4	*g*	..*m*	* *Pbam g*	$b..\ C2xy$
4	*h*			$00\frac{1}{2}\ b..\ C2xy$
8	*i*	1	* *Pbam i*	$b..\ C2xy2z$

56 *Pccn*

4	*a*	$\bar{1}$	*Fmmm a*	F
4	*b*			$00\frac{1}{2}\ F$
4	*c*	..2	*Pmmn a*	$\frac{1}{4}\frac{1}{4}0\ (2_1..\ CI1z)_c$
4	*d*			$\frac{1}{4}\frac{3}{4}0\ (2_1..\ CI1z)_c$
8	*e*	1	* *Pccn e*	$c.2\ F2xyz$

57 *Pbcm*

4	*a*	$\bar{1}$	*Pmmm a*	P_{bc}
4	*b*			$\frac{1}{2}00\ P_{bc}$
4	*c*	2..	*Pmma e*	$0\frac{1}{4}0\ (..2\ P_bC1x)_c$
4	*d*	..*m*	* *Pbcm d*	$00\frac{1}{4}\ 2.\bar{1}\ P_{bc}A_bC_cF1xy$
8	*e*	1	* *Pbcm e*	$2.m\ P_{bc}2xyz$

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

58 *Pnnm*

2	*a*	..2/*m*	*Immm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*			$0\frac{1}{2}0$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *I*
4	*e*	..2	*Immm e*	*I*2*z*
4	*f*			$0\frac{1}{2}0$ *I*2*z*
4	*g*	..*m*	* *Pnnm g*	*n*.. *I*2*xy*
8	*h*	1	* *Pnnm h*	*n*.. *I*2*xy*2*z*

59 *Pmmn*

2	*a*	*mm*2	* *Pmmn a*	2_1.. *CI*1*z*
2	*b*			$0\frac{1}{2}0$ 2_1.. *CI*1*z*
4	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*e*	*m*..	* *Pmmn e*	2_1.. *CI*1*z*2*y*
4	*f*	.*m*.		.2_1. *CI*1*z*2*x*
8	*g*	1	* *Pmmn g*	$\frac{1}{4}\frac{1}{4}0$ *mm*. P_{ab}2*xyz*

60 *Pbcn*

4	*a*	$\bar{1}$	*Cmmm a*	C_c
4	*b*			$0\frac{1}{2}0$ C_c
4	*c*	.2.	*Cmcm c*	$00\frac{1}{4}$ 2_1.. C_cF1*y*
8	*d*	1	* *Pbcn d*	*b*2. C_c2*xyz*

61 *Pbca*

4	*a*	$\bar{1}$	*Fmmm a*	*F*
4	*b*			$00\frac{1}{2}$ *F*
8	*c*	1	* *Pbca c*	*bc*. *F*2*xyz*

62 *Pnma*

4	*a*	$\bar{1}$	*Cmmm a*	B_b
4	*b*			$00\frac{1}{2}$ B_b
4	*c*	.*m*.	* *Pnma c*	$0\frac{1}{4}0$ $\bar{1}$.2_1 $B_bA_aFI_a$1*xz*
8	*d*	1	* *Pnma d*	.*ma* B_b2*xyz*

63 *Cmcm*

4	*a*	2/*m*..	*Cmmm a*	C_c
4	*b*			$0\frac{1}{2}0$ C_c
4	*c*	*m*2*m*	* *Cmcm c*	$00\frac{1}{4}$ 2_1.. C_cF1*y*
8	*d*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	2..	*Cmmm g*	C_c2*x*
8	*f*	*m*..	* *Cmcm f*	.*n*. C_c2*yz*
8	*g*	..*m*	* *Cmcm g*	$00\frac{1}{4}$ 2_1.. C_cF1*y*2*x*
16	*h*	1	* *Cmcm h*	.*n*. C_c2*yz*2*x*

64 *Cmce*

4	*a*	2/*m*..	*Fmmm a*	*F*
4	*b*			$00\frac{1}{2}$ *F*
8	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*d*	2..	*Fmmm g*	*F*2*x*
8	*e*	.2.	*Pmma e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $(2..\ P_cA1y)_{ab}$
8	*f*	*m*..	* *Cmce f*	.2. *F*2*yz*
16	*g*	1	* *Cmce g*	.2. *F*2*yz*2*x*

65 *Cmmm*

2	*a*	*mmm*	* *Cmmm a*	*C*
2	*b*			$\frac{1}{2}00$ *C*
2	*c*			$\frac{1}{2}0\frac{1}{2}$ *C*
2	*d*			$00\frac{1}{2}$ *C*
4	*e*	..2/*m*	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	2*mm*	* *Cmmm g*	*C*2*x*
4	*h*			$00\frac{1}{2}$ *C*2*x*
4	*i*	*m*2*m*		*C*2*y*
4	*j*			$00\frac{1}{2}$ *C*2*y*
4	*k*	*mm*2	* *Cmmm k*	*C*2*z*
4	*l*			$0\frac{1}{2}0$ *C*2*z*
8	*m*	..2	*Pmmm i*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}2*z*
8	*n*	*m*..	* *Cmmm n*	*C*2*y*2*z*
8	*o*	.*m*.		*C*2*x*2*z*
8	*p*	..*m*	* *Cmmm p*	*C*2*x*2*y*
8	*q*			$00\frac{1}{2}$ *C*2*x*2*y*
16	*r*	1	* *Cmmm r*	*C*2*x*2*y*2*z*

66 *Cccm*

4	*a*	222	*Cmmm a*	$00\frac{1}{4}$ C_c
4	*b*			$0\frac{1}{2}\frac{1}{4}$ C_c
4	*c*	..2/*m*	*Cmmm a*	C_c
4	*d*			$0\frac{1}{2}0$ C_c
4	*e*	..2/*m*	*Fmmm a*	$\frac{1}{4}\frac{1}{4}0$ *F*
4	*f*			$\frac{1}{4}\frac{3}{4}0$ *F*
8	*g*	2..	*Cmmm g*	$00\frac{1}{4}$ C_c2*x*
8	*h*	.2.		$00\frac{1}{4}$ C_c2*y*
8	*i*	..2	*Cmmm k*	C_c2*z*
8	*j*			$0\frac{1}{2}0$ C_c2*z*
8	*k*	..2	*Fmmm g*	$\frac{1}{4}\frac{1}{4}0$ *F*2*z*
8	*l*	..*m*	* *Cccm l*	*c*.. C_c2*xy*
16	*m*	1	* *Cccm m*	*c*.. C_c2*xy*2*z*

67 *Cmme*

4	*a*	222	*Pmmm a*	$\frac{1}{4}00$ P_{ab}
4	*b*			$\frac{1}{4}0\frac{1}{2}$ P_{ab}
4	*c*	2/*m*..	*Pmmm a*	P_{ab}
4	*d*			$00\frac{1}{2}$ P_{ab}
4	*e*	.2/*m*.		$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	*mm*2	* *Cmme g*	$0\frac{1}{4}0$ 2.. $P_{ab}F$1*z*
8	*h*	2..	*Pmmm i*	P_{ab}2*x*
8	*i*			$00\frac{1}{2}$ P_{ab}2*x*
8	*j*	.2.		$\frac{1}{4}00$ P_{ab}2*y*
8	*k*			$\frac{1}{4}0\frac{1}{2}$ P_{ab}2*y*
8	*l*	..2	*Pmmm i*	$\frac{1}{4}00$ P_{ab}2*z*
8	*m*	*m*..	* *Cmme m*	.*m*. P_{ab}2*yz*
8	*n*	.*m*.		$0\frac{1}{4}0$ *m*.. P_{ab}2*xz*
16	*o*	1	* *Cmme o*	.*m*. P_{ab}2*yz*2*x*

68 *Ccce*

4	*a*	222	*Fmmm a*	*F*
4	*b*			$00\frac{1}{2}$ *F*
8	*c*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}0\frac{1}{4}$ P_2
8	*d*			$0\frac{1}{4}\frac{1}{4}$ P_2
8	*e*	2..	*Fmmm g*	*F*2*x*
8	*f*	.2.		*F*2*y*
8	*g*	..2	*Fmmm g*	*F*2*z*
8	*h*	..2	*Cmme g*	$\frac{1}{4}\frac{1}{4}0$ $(2..\ P_{ab}F1z)_c$

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

16	*i*	1	* *Ccce i*	*c.. F2x2yz*
69	***Fmmm***			
4	*a*	*mmm*	* *Fmmm a*	*F*
4	*b*			$00\frac{1}{2}$ *F*
8	*c*	2/*m*..	*Pmmm a*	$0\frac{1}{4}\frac{1}{4}$ P_2
8	*d*	.2/*m*.		$\frac{1}{4}0\frac{1}{4}$ P_2
8	*e*	..2/*m*		$\frac{1}{4}\frac{1}{4}0$ P_2
8	*f*	222	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2*mm*	* *Fmmm g*	*F*2*x*
8	*h*	*m*2*m*		*F*2*y*
8	*i*	*mm*2		*F*2*z*
16	*j*	..2	*Pmmm i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2 2z$
16	*k*	.2.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2 2y$
16	*l*	2..		$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2 2x$
16	*m*	*m*..	* *Fmmm m*	*F*2*y*2*z*
16	*n*	.*m*.		*F*2*x*2*z*
16	*o*	..*m*		*F*2*x*2*y*
32	*p*	1	* *Fmmm p*	*F*2*x*2*y*2*z*
70	***Fddd***			
8	*a*	222	* *Fddd a*	*D*
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	$\bar{1}$	* *Fddd c*	*T*
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
16	*e*	2..	* *Fddd e*	*D*2*x*
16	*f*	.2.		*D*2*y*
16	*g*	..2		*D*2*z*
32	*h*	1	* *Fddd h*	*d.. D*2*x*2*yz*
71	***Immm***			
2	*a*	*mmm*	* *Immm a*	*I*
2	*b*			$0\frac{1}{2}\frac{1}{2}$ *I*
2	*c*			$\frac{1}{2}\frac{1}{2}0$ *I*
2	*d*			$\frac{1}{2}0\frac{1}{2}$ *I*
4	*e*	2*mm*	* *Immm e*	*I*2*x*
4	*f*			$0\frac{1}{2}0$ *I*2*x*
4	*g*	*m*2*m*		*I*2*y*
4	*h*			$00\frac{1}{2}$ *I*2*y*
4	*i*	*mm*2		*I*2*z*
4	*j*			$\frac{1}{2}00$ *I*2*z*
8	*k*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*l*	*m*..	* *Immm l*	*I*2*y*2*z*
8	*m*	.*m*.		*I*2*x*2*z*
8	*n*	..*m*		*I*2*x*2*y*
16	*o*	1	* *Immm o*	*I*2*x*2*y*2*z*
72	***Ibam***			
4	*a*	222	*Cmmm a*	$00\frac{1}{4}$ C_c
4	*b*			$\frac{1}{2}0\frac{1}{4}$ C_c
4	*c*	..2/*m*	*Cmmm a*	C_c
4	*d*			$\frac{1}{2}00$ C_c
8	*e*	$\bar{1}$	*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	2..	*Cmmm g*	$00\frac{1}{4}$ $C_c 2x$
8	*g*	.2.		$00\frac{1}{4}$ $C_c 2y$
8	*h*	..2	*Cmmm k*	$C_c 2z$
8	*i*			$0\frac{1}{2}0$ $C_c 2z$
8	*j*	..*m*	* *Ibam j*	*c..* $C_c 2xy$
16	*k*	1	* *Ibam k*	*c..* $C_c 2xy2z$
73	***Ibca***			
8	*a*	$\bar{1}$	*Pmmm a*	P_2
8	*b*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*c*	2..	*Cmme g*	$00\frac{1}{4}$ $(.2.\ P_{bc}F1x)_a$
8	*d*	.2.		$\frac{1}{4}00$ $(..2\ P_{ac}F1y)_b$
8	*e*	..2		$0\frac{1}{4}0$ $(2..\ P_{ab}F1z)_c$
16	*f*	1	* *Ibca f*	22. $P_2 2xyz$
74	***Imma***			
4	*a*	2/*m*..	*Cmmm a*	B_b
4	*b*			$00\frac{1}{2}$ B_b
4	*c*	.2/*m*.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ A_a
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ A_a
4	*e*	*mm*2	* *Imma e*	$0\frac{1}{4}0$ .2. $B_b A_a 1z$
8	*f*	2..	*Cmmm g*	$B_b 2x$
8	*g*	.2.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $A_a 2y$
8	*h*	*m*..	* *Imma h*	.2. $B_b 2yz$
8	*i*	.*m*.		$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. $A_a 2xz$
16	*j*	1	* *Imma j*	.2. $B_b 2yz2x$
75	***P*4**			
1	*a*	4..	*P*4/*mmm a*	*P*[*z*]
1	*b*			$\frac{1}{2}\frac{1}{2}0$ *P*[*z*]
2	*c*	2..	*P*4/*mmm a*	$0\frac{1}{2}0$ *C*[*z*]
4	*d*	1	*P*4/*m j*	*P*4*xy*[*z*]
76	$P4_1$			
4	*a*	1	* $P4_3$ *a*	4_1.. $P_{cc}{}^{v}DI_c 1xy[z]$
77	$P4_2$			
2	*a*	2..	*P*4/*mmm a*	$P_c[z]$
2	*b*			$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
2	*c*	2..	*I*4/*mmm a*	$0\frac{1}{2}0$ *I*[*z*]
4	*d*	1	$P4_2/m$ *j*	$\bar{4}$.. $P_c 2xy[z]$
78	$P4_3$			
4	*a*	1	* $P4_3$ *a*	4_3.. $P_{cc}{}^{v}DI_c 1xy[z]$
79	***I*4**			
2	*a*	4..	*I*4/*mmm a*	*I*[*z*]
4	*b*	2..	*P*4/*mmm a*	$0\frac{1}{2}0$ $C_c[z]$
8	*c*	1	*I*4/*m h*	*I*4*xy*[*z*]
80	$I4_1$			
4	*a*	2..	$I4_1/amd$ *a*	${}^{v}D[z]$
8	*b*	1	* $I4_1$ *b*	4_1.. ${}^{v}D2xy[z]$
81	$P\bar{4}$			
1	*a*	$\bar{4}$..	*P*4/*mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	2..	*P*4/*mmm g*	*P*2*z*
2	*f*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
2	*g*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*h*	1	* $P\bar{4}$ *h*	*P*4*xyz*

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

82 $I\bar{4}$

2	*a*	$\bar{4}..$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*			$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2..	*I*4/*mmm e*	*I*2*z*
4	*f*			$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*g*	1	* $I\bar{4}$ *g*	*I*4*xyz*

83 *P*4/*m*

1	*a*	4/*m*..	*P*4/*mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	2/*m*..	*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*f*			$0\frac{1}{2}\frac{1}{2}$ *C*
2	*g*	4..	*P*4/*mmm g*	*P*2*z*
2	*h*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	*m*..	* *P*4/*m j*	*P*4*xy*
4	*k*			$00\frac{1}{2}$ *P*4*xy*
8	*l*	1	* *P*4/*m l*	*P*4*xy*2*z*

84 $P4_2/m$

2	*a*	2/*m*..	*P*4/*mmm a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	2/*m*..	*I*4/*mmm a*	$0\frac{1}{2}0$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	$\bar{4}..$	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2..	*P*4/*mmm g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..	*I*4/*mmm e*	$0\frac{1}{2}0$ *I*2*z*
4	*j*	*m*..	* $P4_2/m$ *j*	$\bar{4}..$ P_c2xy
8	*k*	1	* $P4_2/m$ *k*	$\bar{4}..$ P_c2xy2z

85 *P*4/*n*

2	*a*	$\bar{4}..$	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	4..	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	$\bar{1}$	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*e*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*f*	2..	*P*4/*mmm g*	*C*2*z*
8	*g*	1	* *P*4/*n g*	$\bar{1}$ *C*4*xyz*

86 $P4_2/n$

2	*a*	$\bar{4}..$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	$\bar{1}$	*I*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
4	*e*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
4	*f*	2..	*I*4/*mmm e*	*I*2*z*
8	*g*	1	* $P4_2/n$ *g*	*n*.. *I*4*xyz*

87 *I*4/*m*

2	*a*	4/*m*..	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2/*m*..	*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}..$	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4..	*I*4/*mmm e*	*I*2*z*
8	*f*	$\bar{1}$	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*..	* *I*4/*m h*	*I*4*xy*
16	*i*	1	* *I*4/*m i*	*I*4*xy*2*z*

88 $I4_1/a$

4	*a*	$\bar{4}..$	$I4_1/amd$ *a*	^{v}D
4	*b*			$00\frac{1}{2}$ ^{v}D
8	*c*	$\bar{1}$	$I4_1/amd$ *c*	^{v}T
8	*d*			$00\frac{1}{2}$ ^{v}T
8	*e*	2..	$I4_1/amd$ *e*	$^{v}D2z$
16	*f*	1	* $I4_1/a$ *f*	*a*.. $^{v}D4xyz$

89 *P*422

1	*a*	422	*P*4/*mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	222.	*P*4/*mmm a*	$\frac{1}{2}00$ *C*
2	*f*			$\frac{1}{2}0\frac{1}{2}$ *C*
2	*g*	4..	*P*4/*mmm g*	*P*2*z*
2	*h*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	..2	*P*4/*mmm j*	*P*4*xx*
4	*k*			$00\frac{1}{2}$ *P*4*xx*
4	*l*	.2.	*P*4/*mmm l*	*P*4*x*
4	*m*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*n*			$00\frac{1}{2}$ *P*4*x*
4	*o*			$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
8	*p*	1	* *P*422 *p*	*P*4*x*2*yz*

90 $P42_12$

2	*a*	2.22	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	4..	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	2..	*P*4/*mmm g*	*C*2*z*
4	*e*	..2	*P*4/*mbm g*	.*b*. *C*2*xx*
4	*f*			$00\frac{1}{2}$.*b*. *C*2*xx*
8	*g*	1	* $P42_12$ *g*	$.2_1.$ *C*2*xx*2*yz*

91 $P4_122$

4	*a*	.2.	* $P4_322$ *a*	$00\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x$
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x$
4	*c*	..2	* $P4_322$ *c*	$00\frac{3}{8}$ $4_1..$ $P_{cc}{}^{v}D1xx$
8	*d*	1	* $P4_322$ *d*	$00\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x2yz$

92 $P4_12_12$

4	*a*	..2	* $P4_32_12$ *a*	$4_1..$ $I_c{}^{v}D1xx$
8	*b*	1	* $P4_32_12$ *b*	$4_1..$ $I_c{}^{v}D1xx2yz$

93 $P4_222$

2	*a*	222.	*P*4/*mmm a*	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	222.	*I*4/*mmm a*	$0\frac{1}{2}0$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	2.22	*P*4/*mmm a*	$00\frac{1}{4}$ P_c

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

2	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2..	$P4/mmm$ *g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..	$I4/mmm$ *e*	$0\frac{1}{2}0$ $I2z$
4	*j*	.2.	$P4_2/mmc$ *j*	..2 P_c2x
4	*k*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ..2 P_c2x
4	*l*			$00\frac{1}{2}$ ..2 P_c2x
4	*m*			$\frac{1}{2}\frac{1}{2}0$ ..2 P_c2x
4	*n*	..2	$P4_2/mcm$ *i*	$00\frac{1}{4}$ .2. P_c2xx
4	*o*			$00\frac{3}{4}$ .2. P_c2xx
8	*p*	1	* $P4_222$ *p*	..2 P_c2x2yz
94	***P*4₂2₁2**			
2	*a*	2.22	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	2..	$I4/mmm$ *e*	$I2z$
4	*d*	2..	$P4/nmm$ *c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
4	*e*	..2	$P4_2/mnm$ *f*	.*n*. $I2xx$
4	*f*			$00\frac{1}{2}$.*n*. $I2xx$
8	*g*	1	* $P4_22_12$ *g*	$.2_1.$ $I2xx2yz$
95	***P*4₃22**			
4	*a*	.2.	* $P4_322$ *a*	$00\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x$
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x$
4	*c*	..2	* $P4_322$ *c*	$00\frac{5}{8}$ $4_3..$ $P_{cc}{}^vD1xx$
8	*d*	1	* $P4_322$ *d*	$00\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x2yz$
96	***P*4₃2₁2**			
4	*a*	..2	* $P4_32_12$ *a*	$4_3..$ $I_c{}^vD1xx$
8	*b*	1	* $P4_32_12$ *b*	$4_3..$ $I_c{}^vD1xx2yz$
97	***I*422**			
2	*a*	422	$I4/mmm$ *a*	I
2	*b*			$00\frac{1}{2}$ I
4	*c*	222.	$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22	$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4..	$I4/mmm$ *e*	$I2z$
8	*f*	2..	$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*g*	..2	$I4/mmm$ *h*	$I4xx$
8	*h*	.2.	$I4/mmm$ *i*	$I4x$
8	*i*			$00\frac{1}{2}$ $I4x$
8	*j*	..2	$I4/mcm$ *h*	$0\frac{1}{2}\frac{1}{4}$.*b*. C_c2xx
16	*k*	1	* $I422$ *k*	$I4x2yz$
98	***I*4₁22**			
4	*a*	2.22	$I4_1/amd$ *a*	${}^vD$
4	*b*			$00\frac{1}{2}$ ${}^vD$
8	*c*	2..	$I4_1/amd$ *e*	${}^vD2z$
8	*d*	..2	* $I4_122$ *d*	.2. ${}^vD2xx$
8	*e*			.2. ${}^vD2x\bar{x}$
8	*f*	.2.	* $I4_122$ *f*	..22 ${}^vTC_{cc}1x$
16	*g*	1	* $I4_122$ *g*	.2. ${}^vD2xx2yz$
99	***P*4*mm***			
1	*a*	4*mm*	$P4/mmm$ *a*	$P[z]$
1	*b*			$\frac{1}{2}\frac{1}{2}0$ $P[z]$
2	*c*	2*mm*.	$P4/mmm$ *a*	$\frac{1}{2}00$ $C[z]$
4	*d*	..*m*	$P4/mmm$ *j*	$P4xx[z]$
4	*e*	.*m*.	$P4/mmm$ *l*	$P4x[z]$
4	*f*			$\frac{1}{2}\frac{1}{2}0$ $P4x[z]$
8	*g*	1	$P4/mmm$ *p*	$P4x2y[z]$
100	***P*4*bm***			
2	*a*	4..	$P4/mmm$ *a*	$C[z]$
2	*b*	2.*mm*	$P4/mmm$ *a*	$\frac{1}{2}00$ $C[z]$
4	*c*	..*m*	$P4/mbm$ *g*	$0\frac{1}{2}0$.*b*. $C2xx[z]$
8	*d*	1	$P4/mbm$ *i*	..*m* $C4xy[z]$
101	***P*4₂*cm***			
2	*a*	2.*mm*	$P4/mmm$ *a*	$P_c[z]$
2	*b*			$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
4	*c*	2..	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
4	*d*	..*m*	$P4_2/mcm$ *i*	.2. $P_c2xx[z]$
8	*e*	1	$P4_2/mcm$ *n*	.2. $P_c2xx2y[z]$
102	***P*4₂*nm***			
2	*a*	2.*mm*	$I4/mmm$ *a*	$I[z]$
4	*b*	2..	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
4	*c*	..*m*	$P4_2/mnm$ *f*	.*n*. $I2xx[z]$
8	*d*	1	$P4_2/mnm$ *i*	.*n*. $I2xx2y[z]$
103	***P*4*cc***			
2	*a*	4..	$P4/mmm$ *a*	$P_c[z]$
2	*b*			$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
4	*c*	2..	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
8	*d*	1	$P4/mcc$ *m*	.*c*. $P_c4xy[z]$
104	***P*4*nc***			
2	*a*	4..	$I4/mmm$ *a*	$I[z]$
4	*b*	2..	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
8	*c*	1	$P4/mnc$ *h*	..2 $I4xy[z]$
105	***P*4₂*mc***			
2	*a*	2*mm*.	$P4/mmm$ *a*	$P_c[z]$
2	*b*			$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
2	*c*	2*mm*.	$I4/mmm$ *a*	$0\frac{1}{2}0$ $I[z]$
4	*d*	.*m*.	$P4_2/mmc$ *j*	..2 $P_c2x[z]$
4	*e*			$\frac{1}{2}\frac{1}{2}0$ ..2 $P_c2x[z]$
8	*f*	1	$P4_2/mmc$ *q*	..2 $P_c2x2y[z]$
106	***P*4₂*bc***			
4	*a*	2..	$P4/mmm$ *a*	$C_c[z]$
4	*b*	2..	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
8	*c*	1	$P4_2/mbc$ *h*	.*b*2 $C_c2xy[z]$
107	***I*4*mm***			
2	*a*	4*mm*	$I4/mmm$ *a*	$I[z]$
4	*b*	2*mm*.	$P4/mmm$ *a*	$0\frac{1}{2}0$ $C_c[z]$
8	*c*	..*m*	$I4/mmm$ *h*	$I4xx[z]$
8	*d*	.*m*.	$I4/mmm$ *i*	$I4x[z]$
16	*e*	1	$I4/mmm$ *l*	$I4x2y[z]$
108	***I*4*cm***			
4	*a*	4..	$P4/mmm$ *a*	$C_c[z]$
4	*b*	2.*mm*	$P4/mmm$ *a*	$\frac{1}{2}00$ $C_c[z]$

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

8	*c*	..*m*	*I*4/*mcm h*	$\frac{1}{2}00$.*b*. $C_c2xx[z]$
16	*d*	1	*I*4/*mcm k*	..*m* $C_c4xy[z]$

109 $I4_1md$

4	*a*	2*mm*.	$I4_1/amd$ *a*	$^vD[z]$
8	*b*	.*m*.	* $I4_1md$ *b*	..*d* $^vD2x[z]$
16	*c*	1	* $I4_1md$ *c*	..*d* $^vD2x2y[z]$

110 $I4_1cd$

8	*a*	2..	*I*4/*mmm a*	$F_c[z]$
16	*b*	1	* $I4_1cd$ *b*	.*bd* $F_c2xy[z]$

111 $P\bar{4}2m$

1	*a*	$\bar{4}2m$	*P*4/*mmm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*c*			$00\frac{1}{2}$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}0$ *P*
2	*e*	222.	*P*4/*mmm a*	$\frac{1}{2}00$ *C*
2	*f*			$\frac{1}{2}0\frac{1}{2}$ *C*
2	*g*	2.*mm*	*P*4/*mmm g*	*P*2*z*
2	*h*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	.2.	*P*4/*mmm l*	*P*4*x*
4	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*k*			$00\frac{1}{2}$ *P*4*x*
4	*l*			$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
4	*m*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*n*	..*m*	* $P\bar{4}2m$ *n*	*P*4*xxz*
8	*o*	1	* $P\bar{4}2m$ *o*	*P*4*xxz*2*y*

112 $P\bar{4}2c$

2	*a*	222.	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	222.	*I*4/*mmm a*	$\frac{1}{2}0\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{4}$ *I*
2	*e*	$\bar{4}$..	*P*4/*mmm a*	P_c
2	*f*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*g*	.2.	$P4_2/mmc$ *j*	$00\frac{1}{4}$ ..2 P_c2x
4	*h*			$\frac{1}{2}\frac{1}{2}\frac{3}{4}$ ..2 P_c2x
4	*i*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ ..2 P_c2x
4	*j*			$00\frac{3}{4}$ ..2 P_c2x
4	*k*	2..	*P*4/*mmm g*	P_c2z
4	*l*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*m*	2..	*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*n*	1	* $P\bar{4}2c$ *n*	.2. P_c4xyz

113 $P\bar{4}2_1m$

2	*a*	$\bar{4}$..	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	2.*mm*	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	2..	*P*4/*mmm g*	*C*2*z*
4	*e*	..*m*	* $P\bar{4}2_1m$ *e*	$0\frac{1}{2}0$ $.2_1.$ *CI*1*z*2*xx*
8	*f*	1	* $P\bar{4}2_1m$ *f*	..*m* *C*4*xyz*

114 $P\bar{4}2_1c$

2	*a*	$\bar{4}$..	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2..	*I*4/*mmm e*	*I*2*z*
4	*d*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*e*	1	* $P\bar{4}2_1c$ *e*	..*c* *I*4*xyz*

115 $P\bar{4}m2$

1	*a*	$\bar{4}m2$	*P*4/*mmm a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*d*			$00\frac{1}{2}$ *P*
2	*e*	2*mm*.	*P*4/*mmm g*	*P*2*z*
2	*f*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
2	*g*	2*mm*.	*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*h*	..2	*P*4/*mmm j*	*P*4*xx*
4	*i*			$00\frac{1}{2}$ *P*4*xx*
4	*j*	.*m*.	* $P\bar{4}m2$ *j*	*P*4*xz*
4	*k*			$\frac{1}{2}\frac{1}{2}0$ *P*4*xz*
8	*l*	1	* $P\bar{4}m2$ *l*	*P*4*xz*2*y*

116 $P\bar{4}c2$

2	*a*	2.22	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*c*	$\bar{4}$..	*P*4/*mmm a*	P_c
2	*d*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	..2	$P4_2/mcm$ *i*	$00\frac{1}{4}$ .2. P_c2xx
4	*f*			$00\frac{3}{4}$ .2. P_c2xx
4	*g*	2..	*P*4/*mmm g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*j*	1	* $P\bar{4}c2$ *j*	..2 P_c4xyz

117 $P\bar{4}b2$

2	*a*	$\bar{4}$..	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	2.22	*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	2..	*P*4/*mmm g*	*C*2*z*
4	*f*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*g*	..2	*P*4/*mbm g*	$0\frac{1}{2}0$.*b*. *C*2*xx*
4	*h*			$0\frac{1}{2}\frac{1}{2}$.*b*. *C*2*xx*
8	*i*	1	* $P\bar{4}b2$ *i*	..2 *C*4*xyz*

118 $P\bar{4}n2$

2	*a*	$\bar{4}$..	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*	2.22	*I*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2..	*I*4/*mmm e*	*I*2*z*
4	*f*	..2	$P4_2/mnm$ *f*	$\frac{1}{2}0\frac{3}{4}$.*n*. *I*2*xx*
4	*g*			$0\frac{1}{2}\frac{1}{4}$.*n*. *I*2*xx*
4	*h*	2..	*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*i*	1	* $P\bar{4}n2$ *i*	..2 *I*4*xyz*

119 $I\bar{4}m2$

2	*a*	$\bar{4}m2$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
2	*c*			$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*			$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2*mm*.	*I*4/*mmm e*	*I*2*z*
4	*f*			$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*g*	..2	*I*4/*mmm h*	*I*4*xx*

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

8	*h*			$0\frac{1}{2}\frac{1}{4}$ *I*4*xx*
8	*i*	.*m*.	* $I\bar{4}m2$ *i*	*I*4*xz*
16	*j*	1	* $I\bar{4}m2$ *j*	*I*4*xz*2*y*

120 $I\bar{4}c2$

4	*a*	2.22	*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*d*			$0\frac{1}{2}0$ C_c
4	*b*	$\bar{4}$..	*P*4/*mmm a*	C_c
4	*c*			$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	..2	*I*4/*mcm h*	$00\frac{1}{4}$.*b*. C_c2xx
8	*h*			$0\frac{1}{2}0$.*b*. C_c2xx
8	*f*	2..	*P*4/*mmm g*	C_c2z
8	*g*			$0\frac{1}{2}0$ C_c2z
16	*i*	1	* $I\bar{4}c2$ *i*	..2 C_c4xyz

121 $I\bar{4}2m$

2	*a*	$\bar{4}2m$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	222.	*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	2.*mm*	*I*4/*mmm e*	*I*2*z*
8	*f*	.2.	*I*4/*mmm i*	*I*4*x*
8	*g*			$00\frac{1}{2}$ *I*4*x*
8	*h*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*i*	..*m*	* $I\bar{4}2m$ *i*	*I*4*xxz*
16	*j*	1	* $I\bar{4}2m$ *j*	*I*4*xxz*2*y*

122 $I\bar{4}2d$

4	*a*	$\bar{4}$..	$I4_1/amd$ *a*	^{v}D
4	*b*			$00\frac{1}{2}$ ^{v}D
8	*c*	2..	$I4_1/amd$ *e*	$^{v}D2z$
8	*d*	.2.	* $I\bar{4}2d$ *d*	$\bar{4}$.. $^{v}TF_c1x$
16	*e*	1	* $I\bar{4}2d$ *e*	.2. $^{v}D4xyz$

123 *P*4/*mmm*

1	*a*	4/*mmm*	* *P*4/*mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
1	*c*			$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	*mmm*.	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{2}$ *C*
2	*f*			$0\frac{1}{2}0$ *C*
2	*g*	4*mm*	* *P*4/*mmm g*	*P*2*z*
2	*h*			$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2*mm*.	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	*m*.2*m*	* *P*4/*mmm j*	*P*4*xx*
4	*k*			$00\frac{1}{2}$ *P*4*xx*
4	*l*	*m*2*m*.	* *P*4/*mmm l*	*P*4*x*
4	*m*			$00\frac{1}{2}$ *P*4*x*
4	*n*			$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
4	*o*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
8	*p*	*m*..	* *P*4/*mmm p*	*P*4*x*2*y*
8	*q*			$00\frac{1}{2}$ *P*4*x*2*y*
8	*r*	..*m*	* *P*4/*mmm r*	*P*4*xx*2*z*
8	*s*	.*m*.	* *P*4/*mmm s*	*P*4*x*2*z*
8	*t*			$\frac{1}{2}\frac{1}{2}0$ *P*4*x*2*z*
16	*u*	1	* *P*4/*mmm u*	*P*4*x*2*y*2*z*

124 *P*4/*mcc*

2	*a*	422	*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	4/*m*..	*P*4/*mmm a*	P_c
2	*d*			$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	2/*m*..	*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*f*	222.	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*g*	4..	*P*4/*mmm g*	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
8	*i*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*j*	..2	*P*4/*mmm j*	$00\frac{1}{4}$ P_c4xx
8	*k*	.2.	*P*4/*mmm l*	$00\frac{1}{4}$ P_c4x
8	*l*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*m*	*m*..	* *P*4/*mcc m*	.*c*. P_c4xy
16	*n*	1	* *P*4/*mcc n*	.*c*. P_c4xy2z

125 *P*4/*nbm*

2	*a*	422	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	$\bar{4}2m$	*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	..2/*m*	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	4..	*P*4/*mmm g*	*C*2*z*
4	*h*	2.*mm*	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
8	*i*	..2	*P*4/*mmm l*	*C*4*xx*
8	*j*			$00\frac{1}{2}$ *C*4*xx*
8	*k*	.2.	*P*4/*mmm j*	*C*4*x*
8	*l*			$00\frac{1}{2}$ *C*4*x*
8	*m*	..*m*	* *P*4/*nbm m*	$0\frac{1}{2}0$ ..2 *C*4*xxz*
16	*n*	1	* *P*4/*nbm n*	..*m* *C*4*x*2*yz*

126 *P*4/*nnc*

2	*a*	422	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	222.	*P*4/*mmm a*	$\frac{1}{2}00$ C_c
4	*d*	$\bar{4}$..	*P*4/*mmm a*	$\frac{1}{2}0\frac{1}{4}$ C_c
4	*e*	4..	*I*4/*mmm e*	*I*2*z*
8	*f*	$\bar{1}$	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..	*P*4/*mmm g*	$\frac{1}{2}00$ C_c2z
8	*h*	..2	*I*4/*mmm h*	*I*4*xx*
8	*i*	.2.	*I*4/*mmm i*	*I*4*x*
8	*j*			$00\frac{1}{2}$ *I*4*x*
16	*k*	1	* *P*4/*nnc k*	..*c* *I*4*x*2*yz*

127 *P*4/*mbm*

2	*a*	4/*m*..	*P*4/*mmm a*	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	*m*.*mm*	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{2}$ *C*
2	*d*			$0\frac{1}{2}0$ *C*
4	*e*	4..	*P*4/*mmm g*	*C*2*z*
4	*f*	2.*mm*	*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*g*	*m*.2*m*	* *P*4/*mbm g*	$0\frac{1}{2}0$.*b*. *C*2*xx*
4	*h*			$0\frac{1}{2}\frac{1}{2}$.*b*. *C*2*xx*
8	*i*	*m*..	* *P*4/*mbm i*	..*m* *C*4*xy*
8	*j*			$00\frac{1}{2}$ ..*m* *C*4*xy*
8	*k*	..*m*	* *P*4/*mbm k*	$0\frac{1}{2}0$.*b*. *C*2*xx*2*z*
16	*l*	1	* *P*4/*mbm l*	..*m* *C*4*xy*2*z*

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

128 P4/mnc

2	*a*	4/m..	I4/mmm a	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2/m..	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*d*	2.22	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4..	I4/mmm e	I2z
8	*f*	2..	P4/mmm g	$0\frac{1}{2}0$ C_c2z
8	*g*	..2	P4/mbm g	$0\frac{1}{2}\frac{1}{4}$ $(.b.\ C2xx)_c$
8	*h*	m..	* P4/mnc h	..2 I4xy
16	*i*	1	* P4/mnc i	..2 I4xy2z

129 P4/nmm

2	*a*	$\bar{4}m2$	P4/mmm a	*C*
2	*b*			$00\frac{1}{2}$ *C*
2	*c*	4mm	* P4/nmm c	$0\frac{1}{2}0$ ..2 CI1z
4	*d*	..2/m	P4/mmm a	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*e*			$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*f*	2mm.	P4/mmm g	C2z
8	*g*	..2	P4/mmm l	C4xx
8	*h*			$00\frac{1}{2}$ C4xx
8	*i*	.m.	* P4/nmm i	..m C4xz
8	*j*	..m	* P4/nmm j	$0\frac{1}{2}0$ ..2 CI1z4xx
16	*k*	1	* P4/nmm k	..m C4xz2y

130 P4/ncc

4	*a*	2.22	P4/mmm a	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}$..	P4/mmm a	C_c
4	*c*	4..	P4/nmm c	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*d*	$\bar{1}$	P4/mmm a	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	2..	P4/mmm g	C_c2z
8	*f*	..2	I4/mcm h	$00\frac{1}{4}$ .b. C_c2xx
16	*g*	1	* P4/ncc g	..c2 C_c4xyz

131 $P4_2/mmc$

2	*a*	mmm.	P4/mmm a	P_c
2	*b*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	mmm.	I4/mmm a	$0\frac{1}{2}0$ *I*
2	*d*			$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	$\bar{4}m2$	P4/mmm a	$00\frac{1}{4}$ P_c
2	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2mm.	P4/mmm g	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2mm.	I4/mmm e	$0\frac{1}{2}0$ I2z
4	*j*	m2m.	* $P4_2/mmc$ j	..2 P_c2x
4	*k*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ..2 P_c2x
4	*l*			$00\frac{1}{2}$ ..2 P_c2x
4	*m*			$\frac{1}{2}\frac{1}{2}0$ ..2 P_c2x
8	*n*	..2	P4/mmm j	$00\frac{1}{4}$ P_c4xx
8	*o*	.m.	* $P4_2/mmc$ o	..c P_c2x2z
8	*p*			$\frac{1}{2}\frac{1}{2}0$ ..c P_c2x2z
8	*q*	m..	* $P4_2/mmc$ q	..2 P_c2x2y
16	*r*	1	* $P4_2/mmc$ r	..c $P_c2x2y2z$

132 $P4_2/mcm$

2	*a*	m.mm	P4/mmm a	P_c
2	*c*			$\frac{1}{2}\frac{1}{2}0$ P_c
2	*b*	$\bar{4}2m$	P4/mmm a	$00\frac{1}{4}$ P_c
2	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*e*	222.	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*f*	2/m..	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*g*	2.mm	P4/mmm g	P_c2z
4	*h*			$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	m.2m	* $P4_2/mcm$ i	.2. P_c2xx
4	*j*			$00\frac{1}{2}$ .2. P_c2xx
8	*k*	2..	P4/mmm g	$0\frac{1}{2}0$ C_c2z
8	*l*	.2.	P4/mmm l	$00\frac{1}{4}$ P_c4x
8	*m*			$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*n*	m..	* $P4_2/mcm$ n	.2. P_c2xx2y
8	*o*	..m	* $P4_2/mcm$ o	.c. P_c2xx2z
16	*p*	1	* $P4_2/mcm$ p	.c. $P_c2xx2y2z$

133 $P4_2/nbc$

4	*a*	222.	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*b*	222.	P4/mmm a	$00\frac{1}{4}$ C_c
4	*c*	2.22	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..	P4/mmm a	C_c
8	*e*	$\bar{1}$	P4/mmm a	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	2..	P4/mmm g	$0\frac{1}{2}0$ C_c2z
8	*g*	2..	P4/mmm g	C_c2z
8	*h*	.2.	$P4_2/mcm$ i	$00\frac{1}{4}$ ..2 C_c2x
8	*i*			$00\frac{3}{4}$ ..2 C_c2x
8	*j*	..2	I4/mcm h	$0\frac{1}{2}0$ .b. C_c2xx
16	*k*	1	* $P4_2/nbc$ k	.22 C_c4xyz

134 $P4_2/nnm$

2	*a*	$\bar{4}2m$	I4/mmm a	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	222.	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*d*	2.22	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	..2/m	I4/mmm a	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*f*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
4	*g*	2.mm	I4/mmm e	I2z
8	*h*	2..	P4/mmm g	$0\frac{1}{2}0$ C_c2z
8	*i*	.2.	I4/mmm i	I4x
8	*j*			$00\frac{1}{2}$ I4x
8	*k*	..2	$P4_2/mmc$ j	$0\frac{1}{2}\frac{1}{4}$ .2. C_c2xx
8	*l*			$0\frac{1}{2}\frac{3}{4}$ .2. C_c2xx
8	*m*	..m	* $P4_2/nnm$ m	..2 I4xxz
16	*n*	1	* $P4_2/nnm$ n	..2 I4xxz2y

135 $P4_2/mbc$

4	*a*	2/m..	P4/mmm a	C_c
4	*b*	$\bar{4}$..	P4/mmm a	$00\frac{1}{4}$ C_c
4	*c*	2/m..	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*d*	2.22	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	2..	P4/mmm g	C_c2z
8	*f*	2..	P4/mmm g	$0\frac{1}{2}0$ C_c2z
8	*g*	..2	P4/mbm g	$0\frac{1}{2}\frac{1}{4}$ $(.b.\ C2xx)_c$
8	*h*	m..	* $P4_2/mbc$ h	.b2 C_c2xy
16	*i*	1	* $P4_2/mbc$ i	.b2 C_c2xy2z

136 $P4_2/mnm$

2	*a*	m.mm	I4/mmm a	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2/m..	P4/mmm a	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..	P4/mmm a	$0\frac{1}{2}\frac{1}{4}$ C_c

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

4	*e*	2.*mm*	*I*4/*mmm e*	*I*2*z*
4	*f*	*m*.2*m*	* $P4_2/mnm$ *f*	.*n*. *I*2*xx*
4	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$.*n*. *I*2*xx*
8	*h*	2..	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*i*	*m*..	* $P4_2/mnm$ *i*	.*n*. *I*2*xx*2*y*
8	*j*	..*m*	* $P4_2/mnm$ *j*	.*n*. *I*2*xx*2*z*
16	*k*	1	* $P4_2/mnm$ *k*	.*n*. *I*2*xx*2*y*2*z*

137 $P4_2/nmc$

2	*a*	$\bar{4}m2$	*I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	2*mm*.	*I*4/*mmm e*	*I*2*z*
4	*d*	2*mm*.	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*e*	$\bar{1}$	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	..2	*I*4/*mmm h*	*I*4*xx*
8	*g*	.*m*.	* $P4_2/nmc$ *g*	..*c* *I*4*xz*
16	*h*	1	* $P4_2/nmc$ *h*	..*c* *I*4*xz*2*y*

138 $P4_2/ncm$

4	*a*	2.22	*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}$..	*P*4/*mmm a*	C_c
4	*c*	..2/*m*	*I*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*			$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
4	*e*	2.*mm*	*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*f*	2..	*P*4/*mmm g*	C_c2z
8	*g*	..2	$P4_2/mmc$ *j*	$00\frac{1}{4}$ .2. C_c2xx
8	*h*			$00\frac{3}{4}$ .2. C_c2xx
8	*i*	..*m*	* $P4_2/ncm$ *i*	$\frac{1}{4}\frac{3}{4}\frac{1}{4}$ $\bar{4}$.. *F*2*xxz*
16	*j*	1	* $P4_2/ncm$ *j*	..*m*2 C_c4xyz

139 *I*4/*mmm*

2	*a*	4/*mmm*	* *I*4/*mmm a*	*I*
2	*b*			$00\frac{1}{2}$ *I*
4	*c*	*mmm*.	*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}m2$	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4*mm*	* *I*4/*mmm e*	*I*2*z*
8	*f*	..2/*m*	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2*mm*.	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*.2*m*	* *I*4/*mmm h*	*I*4*xx*
8	*i*	*m*2*m*.	* *I*4/*mmm i*	*I*4*x*
8	*j*			$\frac{1}{2}\frac{1}{2}0$ *I*4*x*
16	*k*	..2	*P*4/*mmm l*	$0\frac{1}{2}\frac{1}{4}$ C_c4xx
16	*l*	*m*..	* *I*4/*mmm l*	*I*4*x*2*y*
16	*m*	..*m*	* *I*4/*mmm m*	*I*4*xx*2*z*
16	*n*	.*m*.	* *I*4/*mmm n*	*I*4*x*2*z*
32	*o*	1	* *I*4/*mmm o*	*I*4*x*2*y*2*z*

140 *I*4/*mcm*

4	*a*	422	*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}2m$	*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*c*	4/*m*..	*P*4/*mmm a*	C_c
4	*d*	*m*.*mm*	*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
8	*e*	..2/*m*	*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	4..	*P*4/*mmm g*	C_c2z
8	*g*	2.*mm*	*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*.2*m*	* *I*4/*mcm h*	$0\frac{1}{2}0$.*b*. C_c2xx
16	*i*	..2	*P*4/*mmm l*	$00\frac{1}{4}$ C_c4xx
16	*j*	.2.	*P*4/*mmm j*	$00\frac{1}{4}$ C_c4x
16	*k*	*m*..	* *I*4/*mcm k*	..*m* C_c4xy
16	*l*	..*m*	* *I*4/*mcm l*	$0\frac{1}{2}\frac{1}{4}$.*b*. C_c4xxz
32	*m*	1	* *I*4/*mcm m*	.*c*. C_c4xy2z

141 $I4_1/amd$

4	*a*	$\bar{4}m2$	* $I4_1/amd$ *a*	^vD
4	*b*			$00\frac{1}{2}$ ^vD
8	*c*	.2/*m*.	* $I4_1/amd$ *c*	^vT
8	*d*			$00\frac{1}{2}$ ^vT
8	*e*	2*mm*.	* $I4_1/amd$ *e*	^vD2z
16	*f*	.2.	* $I4_1/amd$ *f*	..2 ^vT2x
16	*g*	..2	* $I4_1/amd$ *g*	^vD4xx
16	*h*	.*m*.	* $I4_1/amd$ *h*	.2. ^vD4xz
32	*i*	1	* $I4_1/amd$ *i*	.2. $^vD4xz2y$

142 $I4_1/acd$

8	*a*	$\bar{4}$..	*I*4/*mmm a*	F_c
8	*b*	2.22	*I*4/*mmm a*	$00\frac{1}{4}$ F_c
16	*c*	$\bar{1}$	*I*4/*mmm a*	$0\frac{1}{4}\frac{1}{8}$ I_2
16	*d*	2..	*I*4/*mmm e*	F_c2z
16	*e*	.2.	* $I4_1/acd$ *e*	$0\frac{1}{4}\frac{3}{8}$ $\bar{4}$.. $I_2P_{c2}1x$
16	*f*	..2	* $I4_1/acd$ *f*	$00\frac{1}{4}$ .2. F_c2xx
32	*g*	1	* $I4_1/acd$ *g*	.22 F_c4xyz

143 *P*3

1	*a*	3..	*P*6/*mmm a*	*P*[*z*]
1	*b*			$\frac{1}{3}\frac{2}{3}0$ *P*[*z*]
1	*c*			$\frac{2}{3}\frac{1}{3}0$ *P*[*z*]
3	*d*	1	$P\bar{6}$ *j*	*P*3*xy*[*z*]

144 $P3_1$

3	*a*	1	* $P3_2$ *a*	3_1.. $P_CR^-Q1xy[z]$

145 $P3_2$

3	*a*	1	* $P3_2$ *a*	3_2.. $P_CR^+Q1xy[z]$

146 *R*3 (Hexagonal axes)

3	*a*	3.	$R\bar{3}m$ *a*	*R*[*z*]
9	*b*	1	* *R*3 *b*	*R*3*xy*[*z*]

146 *R*3 (Rhombohedral axes)

1	*a*	3.	$R\bar{3}m$ *a*	*P*[*xxx*]
3	*b*	1	* *R*3 *b*	*P*3*yz*[*xxx*]

147 $P\bar{3}$

1	*a*	$\bar{3}$..	*P*6/*mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
2	*c*	3..	*P*6/*mmm e*	*P*2*z*
2	*d*	3..	$P\bar{3}m1$ *d*	.2. *GE*1*z*
3	*e*	$\bar{1}$	*P*6/*mmm f*	*N*
3	*f*			$00\frac{1}{2}$ *N*
6	*g*	1	* $P\bar{3}$ *g*	*P*6*xyz*

148 $R\bar{3}$ (Hexagonal axes)

3	*a*	$\bar{3}$.	$R\bar{3}m$ *a*	*R*
3	*b*			$00\frac{1}{2}$ *R*
6	*c*	3.	$R\bar{3}m$ *c*	*R*2*z*
9	*d*	$\bar{1}$	$R\bar{3}m$ *e*	$00\frac{1}{2}$ *M*

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

9	*e*			*M*
18	*f*	1	* $R\bar{3}f$	*R6xyz*
148	***R*$\bar{3}$**		(Rhombohedral axes)	
1	*a*	$\bar{3}$.	$R\bar{3}m\ a$	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*c*	3.	$R\bar{3}m\ c$	*P2xxx*
3	*d*	$\bar{1}$	$R\bar{3}m\ e$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
3	*e*			*J*
6	*f*	1	* $R\bar{3}f$	*P6xyz*
149	***P*312**			
1	*a*	3.2	*P6/mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
1	*c*			$\frac{1}{3}\frac{2}{3}0$ *P*
1	*d*			$\frac{1}{3}\frac{2}{3}\frac{1}{2}$ *P*
1	*e*			$\frac{2}{3}\frac{1}{3}0$ *P*
1	*f*			$\frac{2}{3}\frac{1}{3}\frac{1}{2}$ *P*
2	*g*	3..	*P6/mmm e*	*P2z*
2	*h*			$\frac{1}{3}\frac{2}{3}0$ *P2z*
2	*i*			$\frac{2}{3}\frac{1}{3}0$ *P2z*
3	*j*	..2	$P\bar{6}m2\ j$	$P3x\bar{x}$
3	*k*			$00\frac{1}{2}$ $P3x\bar{x}$
6	*l*	1	* *P312 l*	$P3x\bar{x}2yz$
150	***P*321**			
1	*a*	32.	*P6/mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
2	*c*	3..	*P6/mmm e*	*P2z*
2	*d*	3..	$P\bar{3}m1\ d$	*.2. GE1z*
3	*e*	.2.	$P\bar{6}2m\ f$	*P3x*
3	*f*			$00\frac{1}{2}$ *P3x*
6	*g*	1	* *P321 g*	*P3x2yz*
151	***P*3$_1$12**			
3	*a*	..2	* $P3_212\ a$	$00\frac{1}{3}$ 3_1.. $P_C{}^-Q1x\bar{x}$
3	*b*			$00\frac{5}{6}$ 3_1.. $P_C{}^-Q1x\bar{x}$
6	*c*	1	* $P3_212\ c$	$00\frac{1}{3}$ 3_1.. $P_C{}^-Q1x\bar{x}2yz$
152	***P*3$_1$21**			
3	*a*	.2.	* $P3_221\ a$	$00\frac{1}{3}$ 3_1.. P_CR^-Q1x
3	*b*			$00\frac{5}{6}$ 3_1.. P_CR^-Q1x
6	*c*	1	* $P3_221\ c$	$00\frac{1}{3}$ 3_1.. $P_CR^-Q1x2yz$
153	***P*3$_2$12**			
3	*a*	..2	* $P3_212\ a$	$00\frac{2}{3}$ 3_2.. $P_C{}^+Q1x\bar{x}$
3	*b*			$00\frac{1}{6}$ 3_2.. $P_C{}^+Q1x\bar{x}$
6	*c*	1	* $P3_212\ c$	$00\frac{2}{3}$ 3_2.. $P_C{}^+Q1x\bar{x}2yz$
154	***P*3$_2$21**			
3	*a*	.2.	* $P3_221\ a$	$00\frac{2}{3}$ 3_2.. P_CR^+Q1x
3	*b*			$00\frac{1}{6}$ 3_2.. P_CR^+Q1x
6	*c*	1	* $P3_221\ c$	$00\frac{2}{3}$ 3_2.. $P_CR^+Q1x2yz$
155	***R*32**		(Hexagonal axes)	
3	*a*	32	$R\bar{3}m\ a$	*R*
3	*b*			$00\frac{1}{2}$ *R*
6	*c*	3.	$R\bar{3}m\ c$	*R2z*
9	*d*	.2	* *R32 d*	*R3x*
9	*e*			$00\frac{1}{2}$ *R3x*
18	*f*	1	* *R32 f*	*R3x2yz*
155	***R*32**		(Rhombohedral axes)	
1	*a*	32	$R\bar{3}m\ a$	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*c*	3.	$R\bar{3}m\ c$	*P2xxx*
3	*d*	.2	* *R32 d*	$P3x\bar{x}$
3	*e*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $P3x\bar{x}$
6	*f*	1	* *R32 f*	$P3x\bar{x}2yz$
156	***P*3*m*1**			
1	*a*	3*m*.	*P6/mmm a*	*P*[*z*]
1	*b*			$\frac{1}{3}\frac{2}{3}0$ *P*[*z*]
1	*c*			$\frac{2}{3}\frac{1}{3}0$ *P*[*z*]
3	*d*	.*m*.	$P\bar{6}m2\ j$	$P3x\bar{x}$[*z*]
6	*e*	1	$P\bar{6}m2\ l$	$P3x\bar{x}2y$[*z*]
157	***P*31*m***			
1	*a*	3.*m*	*P6/mmm a*	*P*[*z*]
2	*b*	3..	*P6/mmm c*	*G*[*z*]
3	*c*	..*m*	$P\bar{6}2m\ f$	*P3x*[*z*]
6	*d*	1	$P\bar{6}2m\ j$	*P3x2y*[*z*]
158	***P*3*c*1**			
2	*a*	3..	*P6/mmm a*	P_c[*z*]
2	*b*			$\frac{1}{3}\frac{2}{3}0$ P_c[*z*]
2	*c*			$\frac{2}{3}\frac{1}{3}0$ P_c[*z*]
6	*d*	1	$P\bar{6}c2\ k$	..2 P_c3xy[*z*]
159	***P*31*c***			
2	*a*	3..	*P6/mmm a*	P_c[*z*]
2	*b*	3..	$P6_3/mmc\ c$	*E*[*z*]
6	*c*	1	$P\bar{6}2c\ h$	.2. P_c3xy[*z*]
160	***R*3*m***		(Hexagonal axes)	
3	*a*	3*m*	$R\bar{3}m\ a$	*R*[*z*]
9	*b*	.*m*	* *R3m b*	$R3x\bar{x}$[*z*]
18	*c*	1	* *R3m c*	$R3x\bar{x}2y$[*z*]
160	***R*3*m***		(Rhombohedral axes)	
1	*a*	3*m*	$R\bar{3}m\ a$	*P*[*xxx*]
3	*b*	.*m*	* *R3m b*	*P3z*[*xxx*]
6	*c*	1	* *R3m c*	*P3z2y*[*xxx*]
161	***R*3*c***		(Hexagonal axes)	
6	*a*	3.	$R\bar{3}m\ a$	$'R_c$[*z*]
18	*b*	1	* *R3c b*	.*c* $'R_c3xy$[*z*]
161	***R*3*c***		(Rhombohedral axes)	
2	*a*	3.	$R\bar{3}m\ a$	*I*[*xxx*]
6	*b*	1	* *R3c b*	.*n* *I3yz*[*xxx*]
162	***P*$\bar{3}$1*m***			
1	*a*	$\bar{3}$.*m*	*P6/mmm a*	*P*
1	*b*			$00\frac{1}{2}$ *P*
2	*c*	3.2	*P6/mmm c*	*G*

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

2	*d*			$00\frac{1}{2}\,G$
2	*e*	$3.m$	$P6/mmm\ e$	$P2z$
3	*f*	$..2/m$	$P6/mmm\ f$	N
3	*g*			$00\frac{1}{2}\,N$
4	*h*	$3..$	$P6/mmm\ h$	$G2z$
6	*i*	$..2$	$P6/mmm\ l$	$P6x\bar{x}$
6	*j*			$00\frac{1}{2}\,P6x\bar{x}$
6	*k*	$..m$	$^*\,P\bar{3}1m\ k$	$P6xz$
12	*l*	1	$^*\,P\bar{3}1m\ l$	$P6xz2y$
163	$\boldsymbol{P\bar{3}1c}$			
2	*a*	3.2	$P6/mmm\ a$	$00\frac{1}{4}\,P_c$
2	*b*	$\bar{3}..$	$P6/mmm\ a$	P_c
2	*c*	3.2	$P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\,E$
4	*e*	$3..$	$P6/mmm\ e$	P_c2z
4	*f*	$3..$	$P6_3/mmc\ f$	$E2z$
6	*g*	$\bar{1}$	$P6/mmm\ f$	N_c
6	*h*	$..2$	$P6_3/mmc\ h$	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$
12	*i*	1	$^*\,P\bar{3}1c\ i$	$..c\ P_c6xyz$
164	$\boldsymbol{P\bar{3}m1}$			
1	*a*	$\bar{3}m.$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\,P$
2	*c*	$3m.$	$P6/mmm\ e$	$P2z$
2	*d*	$3m.$	$^*\,P\bar{3}m1\ d$	$.2.\ GE1z$
3	*e*	$.2/m.$	$P6/mmm\ f$	N
3	*f*			$00\frac{1}{2}\,N$
6	*g*	$.2.$	$P6/mmm\ j$	$P6x$
6	*h*			$00\frac{1}{2}\,P6x$
6	*i*	$.m.$	$^*\,P\bar{3}m1\ i$	$P6x\bar{x}z$
12	*j*	1	$^*\,P\bar{3}m1\ j$	$P6x\bar{x}z2y$
165	$\boldsymbol{P\bar{3}c1}$			
2	*a*	$32.$	$P6/mmm\ a$	$00\frac{1}{4}\,P_c$
2	*b*	$\bar{3}..$	$P6/mmm\ a$	P_c
4	*c*	$3..$	$P6/mmm\ e$	P_c2z
4	*d*	$3..$	$P\bar{3}m1\ d$	$(.2.\ GE1z)_c$
6	*e*	$\bar{1}$	$P6/mmm\ f$	N_c
6	*f*	$.2.$	$P6_3/mcm\ g$	$00\frac{1}{4}\ ..2\ P_c3x$
12	*g*	1	$^*\,P\bar{3}c1\ g$	$.c.\ P_c6xyz$
166	$\boldsymbol{R\bar{3}m}$	(Hexagonal axes)		
3	*a*	$\bar{3}m$	$^*\,R\bar{3}m\ a$	R
3	*b*			$00\frac{1}{2}\,R$
6	*c*	$3m$	$^*\,R\bar{3}m\ c$	$R2z$
9	*e*	$.2/m$	$^*\,R\bar{3}m\ e$	M
9	*d*			$00\frac{1}{2}\,M$
18	*f*	$.2$	$^*\,R\bar{3}m\ f$	$R6x$
18	*g*			$00\frac{1}{2}\,R6x$
18	*h*	$.m$	$^*\,R\bar{3}m\ h$	$R6x\bar{x}z$
36	*i*	1	$^*\,R\bar{3}m\ i$	$R6x\bar{x}z2y$
166	$\boldsymbol{R\bar{3}m}$	(Rhombohedral axes)		
1	*a*	$\bar{3}m$	$^*\,R\bar{3}m\ a$	P
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\,P$
2	*c*	$3m$	$^*\,R\bar{3}m\ c$	$P2xxx$
3	*e*	$.2/m$	$^*\,R\bar{3}m\ e$	J
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\,J$
6	*f*	$.2$	$^*\,R\bar{3}m\ f$	$P6x\bar{x}$
6	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\,P6x\bar{x}$
6	*h*	$.m$	$^*\,R\bar{3}m\ h$	$P6xxz$
12	*i*	1	$^*\,R\bar{3}m\ i$	$P6xxz2y$
167	$\boldsymbol{R\bar{3}c}$	(Hexagonal axes)		
6	*a*	32	$R\bar{3}m\ a$	$00\frac{1}{4}\,{}'R_c$
6	*b*	$\bar{3}.$	$R\bar{3}m\ a$	${}'R_c$
12	*c*	$3.$	$R\bar{3}m\ c$	${}'R_c2z$
18	*d*	$\bar{1}$	$R\bar{3}m\ e$	${}'M_c$
18	*e*	$.2$	$^*\,R\bar{3}c\ e$	$00\frac{1}{4}\ .c\ {}'R_c3x$
36	*f*	1	$^*\,R\bar{3}c\ f$	$.c\ {}'R_c6xyz$
167	$\boldsymbol{R\bar{3}c}$	(Rhombohedral axes)		
2	*a*	32	$R\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\,I$
2	*b*	$\bar{3}.$	$R\bar{3}m\ a$	I
4	*c*	$3.$	$R\bar{3}m\ c$	$I2xxx$
6	*d*	$\bar{1}$	$R\bar{3}m\ e$	J^*
6	*e*	$.2$	$^*\,R\bar{3}c\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ .n\ I3x\bar{x}$
12	*f*	1	$^*\,R\bar{3}c\ f$	$.n\ I6xyz$
168	$\boldsymbol{P6}$			
1	*a*	$6..$	$P6/mmm\ a$	$P[z]$
2	*b*	$3..$	$P6/mmm\ c$	$G[z]$
3	*c*	$2..$	$P6/mmm\ f$	$N[z]$
6	*d*	1	$P6/m\ j$	$P6xy[z]$
169	$\boldsymbol{P6_1}$			
6	*a*	1	$^*\,P6_1\ a$	$3_12_1..\ P_{C_c}E_C{}^+Q_c1xy[z]$
170	$\boldsymbol{P6_5}$			
6	*a*	1	$^*\,P6_1a$	$3_22_1..\ P_{C_c}E_C{}^-Q_c1xy[z]$
171	$\boldsymbol{P6_2}$			
3	*a*	$2..$	$P6/mmm\ a$	$P_C[z]$
3	*b*	$2..$	$P6_222\ c$	${}^+Q[z]$
6	*c*	1	$^*\,P6_2\ c$	$3_2..\ P_C2xy[z]$
172	$\boldsymbol{P6_4}$			
3	*a*	$2..$	$P6/mmm\ a$	$P_C[z]$
3	*b*	$2..$	$P6_222\ c$	${}^-Q[z]$
6	*c*	1	$^*\,P6_2\ c$	$3_1..\ P_C2xy[z]$
173	$\boldsymbol{P6_3}$			
2	*a*	$3..$	$P6/mmm\ a$	$P_c[z]$
2	*b*	$3..$	$P6_3/mmc\ c$	$E[z]$
6	*c*	1	$P6_3/m\ h$	$2_1..\ P_c3xy[z]$
174	$\boldsymbol{P\bar{6}}$			
1	*a*	$\bar{6}..$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\,P$
1	*c*			$\frac{1}{3}\frac{2}{3}0\,P$
1	*d*			$\frac{1}{3}\frac{2}{3}\frac{1}{2}\,P$
1	*e*			$\frac{2}{3}\frac{1}{3}0\,P$
1	*f*			$\frac{2}{3}\frac{1}{3}\frac{1}{2}\,P$
2	*g*	$3..$	$P6/mmm\ e$	$P2z$
2	*h*			$\frac{1}{3}\frac{2}{3}0\,P2z$

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

2	*i*			$\frac{2}{3}\frac{1}{3}0$ $P2z$
3	*j*	*m..*	* $P\bar{6}$ *j*	$P3xy$
3	*k*			$00\frac{1}{2}$ $P3xy$
6	*l*	1	* $P\bar{6}$ *l*	$P3xy2z$

175 $P6/m$

1	*a*	$6/m..$	$P6/mmm$ *a*	P
1	*b*			$00\frac{1}{2}$ P
2	*c*	$\bar{6}..$	$P6/mmm$ *c*	G
2	*d*			$00\frac{1}{2}$ G
2	*e*	$6..$	$P6/mmm$ *e*	$P2z$
3	*f*	$2/m..$	$P6/mmm$ *f*	N
3	*g*			$00\frac{1}{2}$ N
4	*h*	$3..$	$P6/mmm$ *h*	$G2z$
6	*i*	$2..$	$P6/mmm$ *i*	$N2z$
6	*j*	*m..*	* $P6/m$ *j*	$P6xy$
6	*k*			$00\frac{1}{2}$ $P6xy$
12	*l*	1	* $P6/m$ *l*	$P6xy2z$

176 $P6_3/m$

2	*a*	$\bar{6}..$	$P6/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*b*	$\bar{3}..$	$P6/mmm$ *a*	P_c
2	*c*	$\bar{6}..$	$P6_3/mmc$ *c*	E
2	*d*			$00\frac{1}{2}$ E
4	*e*	$3..$	$P6/mmm$ *e*	P_c2z
4	*f*	$3..$	$P6_3/mmc$ *f*	$E2z$
6	*g*	$\bar{1}$	$P6/mmm$ *f*	N_c
6	*h*	*m..*	* $P6_3/m$ *h*	$00\frac{1}{4}$ $2_1..$ P_c3xy
12	*i*	1	* $P6_3/m$ *i*	$m..$ P_c6xyz

177 $P622$

1	*a*	622	$P6/mmm$ *a*	P
1	*b*			$00\frac{1}{2}$ P
2	*c*	3.2	$P6/mmm$ *c*	G
2	*d*			$00\frac{1}{2}$ G
2	*e*	$6..$	$P6/mmm$ *e*	$P2z$
3	*f*	222	$P6/mmm$ *f*	N
3	*g*			$00\frac{1}{2}$ N
4	*h*	$3..$	$P6/mmm$ *h*	$G2z$
6	*i*	$2..$	$P6/mmm$ *i*	$N2z$
6	*j*	.2.	$P6/mmm$ *j*	$P6x$
6	*k*			$00\frac{1}{2}$ $P6x$
6	*l*	..2	$P6/mmm$ *l*	$P6x\bar{x}$
6	*m*			$00\frac{1}{2}$ $P6x\bar{x}$
12	*n*	1	* $P622$ *n*	$P6x2yz$

178 $P6_122$

6	*a*	.2.	* $P6_122$ *a*	$3_1.2$ $P_{Cc}{}^{+}Q_c1x$
6	*b*	..2	* $P6_122$ *b*	$00\frac{11}{12}$ $3_12.$ $P_{Cc}E_C{}^{+}Q_c1x\bar{x}$
12	*c*	1	* $P6_122$ *c*	$3_1.2$ $P_{Cc}{}^{+}Q_c1x2yz$

179 $P6_522$

6	*a*	.2.	* $P6_122$ *a*	$3_2.2$ $P_{Cc}{}^{-}Q_c1x$
6	*b*	..2	* $P6_122$ *b*	$00\frac{1}{12}$ $3_22.$ $P_{Cc}E_C{}^{-}Q_c1x\bar{x}$
12	*c*	1	* $P6_122$ *c*	$3_2.2$ $P_{Cc}{}^{-}Q_c1x2yz$

180 $P6_222$

3	*a*	222	$P6/mmm$ *a*	P_C
3	*b*			$00\frac{1}{2}$ P_C
3	*c*	222	* $P6_222$ *c*	${}^{+}Q$
3	*d*			$00\frac{1}{2}$ ${}^{+}Q$
6	*e*	$2..$	$P6/mmm$ *e*	P_C2z
6	*f*	$2..$	* $P6_222$ *f*	${}^{+}Q2z$
6	*g*	.2.	* $P6_222$ *g*	$3_2..$ P_C2x
6	*h*			$00\frac{1}{2}$ $3_2..$ P_C2x
6	*i*	..2	* $P6_222$ *i*	$00\frac{1}{3}$ $3_2..$ $P_C2x\bar{x}$
6	*j*			$00\frac{5}{6}$ $3_2..$ $P_C2x\bar{x}$
12	*k*	1	* $P6_222$ *k*	$3_2..$ P_C2x2yz

181 $P6_422$

3	*a*	222	$P6/mmm$ *a*	P_C
3	*b*			$00\frac{1}{2}$ P_C
3	*c*	222	* $P6_222$ *c*	${}^{-}Q$
3	*d*			$00\frac{1}{2}$ ${}^{-}Q$
6	*e*	$2..$	$P6/mmm$ *e*	P_C2z
6	*f*	$2..$	* $P6_222$ *f*	${}^{-}Q2z$
6	*g*	.2.	* $P6_222$ *g*	$3_1..$ P_C2x
6	*h*			$00\frac{1}{2}$ $3_1..$ P_C2x
6	*i*	..2	* $P6_222$ *i*	$00\frac{2}{3}$ $3_1..$ $P_C2x\bar{x}$
6	*j*			$00\frac{1}{6}$ $3_1..$ $P_C2x\bar{x}$
12	*k*	1	* $P6_222$ *k*	$3_1..$ P_C2x2yz

182 $P6_322$

2	*a*	32.	$P6/mmm$ *a*	P_c
2	*b*	3.2	$P6/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*c*	3.2	$P6_3/mmc$ *c*	E
2	*d*			$00\frac{1}{2}$ E
4	*e*	$3..$	$P6/mmm$ *e*	P_c2z
4	*f*	$3..$	$P6_3/mmc$ *f*	$E2z$
6	*g*	.2.	$P6_3/mcm$ *g*	$..2$ P_c3x
6	*h*	..2	$P6_3/mmc$ *h*	$00\frac{1}{4}$ $.2.$ $P_c3x\bar{x}$
12	*i*	1	* $P6_322$ *i*	$..2$ P_c3x2yz

183 $P6mm$

1	*a*	$6mm$	$P6/mmm$ *a*	$P[z]$
2	*b*	$3m.$	$P6/mmm$ *c*	$G[z]$
3	*c*	$2mm$	$P6/mmm$ *f*	$N[z]$
6	*d*	$..m$	$P6/mmm$ *j*	$P6x[z]$
6	*e*	$.m.$	$P6/mmm$ *l*	$P6x\bar{x}[z]$
12	*f*	1	$P6/mmm$ *p*	$P6x2y[z]$

184 $P6cc$

2	*a*	$6..$	$P6/mmm$ *a*	$P_c[z]$
4	*b*	$3..$	$P6/mmm$ *c*	$G_c[z]$
6	*c*	$2..$	$P6/mmm$ *f*	$N_c[z]$
12	*d*	1	$P6/mcc$ *l*	$.c.$ $P_c6xy[z]$

185 $P6_3cm$

2	*a*	$3.m$	$P6/mmm$ *a*	$P_c[z]$
4	*b*	$3..$	$P6/mmm$ *c*	$G_c[z]$
6	*c*	$..m$	$P6_3/mcm$ *g*	$..2$ $P_c3x[z]$
12	*d*	1	$P6_3/mcm$ *j*	$..2$ $P_c3x2y[z]$

186 $P6_3mc$

2	*a*	$3m.$	$P6/mmm$ *a*	$P_c[z]$
2	*b*	$3m.$	$P6_3/mmc$ *c*	$E[z]$

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

6	*c*	.*m*.	$P6_3/mmc\ h$	$.2.\ P_c3x\bar{x}[z]$
12	*d*	1	$P6_3/mmc\ j$	$.2.\ P_c3x\bar{x}2y[z]$

187 $P\bar{6}m2$

1	*a*	$\bar{6}m2$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
1	*c*			$\frac{1}{3}\frac{2}{3}0\ P$
1	*d*			$\frac{1}{3}\frac{2}{3}\frac{1}{2}\ P$
1	*e*			$\frac{2}{3}\frac{1}{3}0\ P$
1	*f*			$\frac{2}{3}\frac{1}{3}\frac{1}{2}\ P$
2	*g*	$3m.$	$P6/mmm\ e$	$P2z$
2	*h*			$\frac{1}{3}\frac{2}{3}0\ P2z$
2	*i*			$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	$mm2$	$^{*}\ P\bar{6}m2\ j$	$P3x\bar{x}$
3	*k*			$00\frac{1}{2}\ P3x\bar{x}$
6	*l*	$m..$	$^{*}\ P\bar{6}m2\ l$	$P3x\bar{x}2y$
6	*m*			$00\frac{1}{2}\ P3x\bar{x}2y$
6	*n*	$.m.$	$^{*}\ P\bar{6}m2\ n$	$P3x\bar{x}2z$
12	*o*	1	$^{*}\ P\bar{6}m2\ o$	$P3x\bar{x}2y2z$

188 $P\bar{6}c2$

2	*a*	3.2	$P6/mmm\ a$	P_c
2	*c*			$\frac{1}{3}\frac{2}{3}0\ P_c$
2	*e*			$\frac{2}{3}\frac{1}{3}0\ P_c$
2	*b*	$\bar{6}..$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*d*			$\frac{1}{3}\frac{2}{3}\frac{1}{4}\ P_c$
2	*f*			$\frac{2}{3}\frac{1}{3}\frac{1}{4}\ P_c$
4	*g*	$3..$	$P6/mmm\ e$	P_c2z
4	*h*			$\frac{1}{3}\frac{2}{3}0\ P_c2z$
4	*i*			$\frac{2}{3}\frac{1}{3}0\ P_c2z$
6	*j*	$..2$	$P\bar{6}m2\ j$	$P_c3x\bar{x}$
6	*k*	$m..$	$^{*}\ P\bar{6}c2\ k$	$00\frac{1}{4}\ ..2\ P_c3xy$
12	*l*	1	$^{*}\ P\bar{6}c2\ l$	$m..\ P_c3x\bar{x}2yz$

189 $P\bar{6}2m$

1	*a*	$\bar{6}2m$	$P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	$\bar{6}..$	$P6/mmm\ c$	G
2	*d*			$00\frac{1}{2}\ G$
2	*e*	$3.m$	$P6/mmm\ e$	$P2z$
3	*f*	$m2m$	$^{*}\ P\bar{6}2m\ f$	$P3x$
3	*g*			$00\frac{1}{2}\ P3x$
4	*h*	$3..$	$P6/mmm\ h$	$G2z$
6	*i*	$..m$	$^{*}\ P\bar{6}2m\ i$	$P3x2z$
6	*j*	$m..$	$^{*}\ P\bar{6}2m\ j$	$P3x2y$
6	*k*			$00\frac{1}{2}\ P3x2y$
12	*l*	1	$^{*}\ P\bar{6}2m\ l$	$P3x2y2z$

190 $P\bar{6}2c$

2	*a*	$32.$	$P6/mmm\ a$	P_c
2	*b*	$\bar{6}..$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*c*	$\bar{6}..$	$P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\ E$
4	*e*	$3..$	$P6/mmm\ e$	P_c2z
4	*f*	$3..$	$P6_3/mmc\ f$	$E2z$
6	*g*	$.2.$	$P\bar{6}2m\ f$	P_c3x
6	*h*	$m..$	$^{*}\ P\bar{6}2c\ h$	$00\frac{1}{4}\ .2.\ P_c3xy$
12	*i*	1	$^{*}\ P\bar{6}2c\ i$	$m..\ P_c3x2yz$

191 $P6/mmm$

1	*a*	$6/mmm$	$^{*}\ P6/mmm\ a$	P
1	*b*			$00\frac{1}{2}\ P$
2	*c*	$\bar{6}m2$	$^{*}\ P6/mmm\ c$	G
2	*d*			$00\frac{1}{2}\ G$
2	*e*	$6mm$	$^{*}\ P6/mmm\ e$	$P2z$
3	*f*	mmm	$^{*}\ P6/mmm\ f$	N
3	*g*			$00\frac{1}{2}\ N$
4	*h*	$3m.$	$^{*}\ P6/mmm\ h$	$G2z$
6	*i*	$2mm$	$^{*}\ P6/mmm\ i$	$N2z$
6	*j*	$m2m$	$^{*}\ P6/mmm\ j$	$P6x$
6	*k*			$00\frac{1}{2}\ P6x$
6	*l*	$mm2$	$^{*}\ P6/mmm\ l$	$P6x\bar{x}$
6	*m*			$00\frac{1}{2}\ P6x\bar{x}$
12	*n*	$..m$	$^{*}\ P6/mmm\ n$	$P6x2z$
12	*o*	$.m.$	$^{*}\ P6/mmm\ o$	$P6x\bar{x}2z$
12	*p*	$m..$	$^{*}\ P6/mmm\ p$	$P6x2y$
12	*q*			$00\frac{1}{2}\ P6x2y$
24	*r*	1	$^{*}\ P6/mmm\ r$	$P6x2y2z$

192 $P6/mcc$

2	*a*	622	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*b*	$6/m..$	$P6/mmm\ a$	P_c
4	*c*	3.2	$P6/mmm\ c$	$00\frac{1}{4}\ G_c$
4	*d*	$\bar{6}..$	$P6/mmm\ c$	G_c
4	*e*	$6..$	$P6/mmm\ e$	P_c2z
6	*f*	222	$P6/mmm\ f$	$00\frac{1}{4}\ N_c$
6	*g*	$2/m..$	$P6/mmm\ f$	N_c
8	*h*	$3..$	$P6/mmm\ h$	G_c2z
12	*i*	$2..$	$P6/mmm\ i$	N_c2z
12	*j*	$.2.$	$P6/mmm\ j$	$00\frac{1}{4}\ P_c6x$
12	*k*	$..2$	$P6/mmm\ l$	$00\frac{1}{4}\ P_c6x\bar{x}$
12	*l*	$m..$	$^{*}\ P6/mcc\ l$	$.c.\ P_c6xy$
24	*m*	1	$^{*}\ P6/mcc\ m$	$.c.\ P_c6xy2z$

193 $P6_3/mcm$

2	*a*	$\bar{6}2m$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}.m$	$P6/mmm\ a$	P_c
4	*c*	$\bar{6}..$	$P6/mmm\ c$	$00\frac{1}{4}\ G_c$
4	*d*	3.2	$P6/mmm\ c$	G_c
4	*e*	$3.m$	$P6/mmm\ e$	P_c2z
6	*f*	$..2/m$	$P6/mmm\ f$	N_c
6	*g*	$m2m$	$^{*}\ P6_3/mcm\ g$	$00\frac{1}{4}\ ..2\ P_c3x$
8	*h*	$3..$	$P6/mmm\ h$	G_c2z
12	*i*	$..2$	$P6/mmm\ l$	$P_c6x\bar{x}$
12	*j*	$m..$	$^{*}\ P6_3/mcm\ j$	$00\frac{1}{4}\ ..2\ P_c3x2y$
12	*k*	$..m$	$^{*}\ P6_3/mcm\ k$	$m..\ P_c6xz$
24	*l*	1	$^{*}\ P6_3/mcm\ l$	$m..\ P_c6xz2y$

194 $P6_3/mmc$

2	*a*	$\bar{3}m.$	$P6/mmm\ a$	P_c
2	*b*	$\bar{6}m2$	$P6/mmm\ a$	$00\frac{1}{4}\ P_c$
2	*c*	$\bar{6}m2$	$^{*}\ P6_3/mmc\ c$	E
2	*d*			$00\frac{1}{2}\ E$
4	*e*	$3m.$	$P6/mmm\ e$	P_c2z
4	*f*	$3m.$	$^{*}\ P6_3/mmc\ f$	$E2z$
6	*g*	$.2/m.$	$P6/mmm\ f$	N_c
6	*h*	$mm2$	$^{*}\ P6_3/mmc\ h$	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$

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

12	*i*	.2.	$P6/mmm$ *j*	P_c6x
12	*j*	*m*..	* $P6_3/mmc$ *j*	$00\frac{1}{4}$ .2. $P_c3x\bar{x}2y$
12	*k*	.*m*.	* $P6_3/mmc$ *k*	*m*.. $P_c6x\bar{x}z$
24	*l*	1	* $P6_3/mmc$ *l*	*m*.. $P_c6x\bar{x}z2y$

195 *P*23

1	*a*	23.	$Pm\bar{3}m$ *a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	222..	$Pm\bar{3}m$ *c*	*J*
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
4	*e*	.3.	$P\bar{4}3m$ *e*	*P*4*xxx*
6	*f*	2..	$Pm\bar{3}m$ *e*	*P*6*z*
6	*i*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*g*	2..	$Pm\bar{3}$ *f*	.3. *J*2*x*
6	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
12	*j*	1	* *P*23 *j*	*P*6*z*2*xy*

196 *F*23

4	*a*	23.	$Fm\bar{3}m$ *a*	*F*
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
4	*c*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
16	*e*	.3.	$F\bar{4}3m$ *e*	*F*4*xxx*
24	*f*	2..	$Fm\bar{3}m$ *e*	*F*6*z*
24	*g*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*6*z*
48	*h*	1	* *F*23 *h*	*F*6*z*2*xy*

197 *I*23

2	*a*	23.	$Im\bar{3}m$ *a*	*I*
6	*b*	222..	$Im\bar{3}m$ *b*	J^*
8	*c*	.3.	$I\bar{4}3m$ *c*	*I*4*xxx*
12	*d*	2..	$Im\bar{3}m$ *e*	*I*6*z*
12	*e*	2..	$Im\bar{3}$ *e*	.3. J^*2x
24	*f*	1	* *I*23 *f*	*I*6*z*2*xy*

198 $P2_13$

4	*a*	.3.	* $P2_13$ *a*	2_12_1.. *FY*1*xxx*
12	*b*	1	* $P2_13$ *b*	2_12_1.. *FY*1*xxx*3*yz*

199 $I2_13$

8	*a*	.3.	* $I2_13$ *a*	2_12_1.. P_2Y^*1xxx
12	*b*	2..	* $I2_13$ *b*	2_13. *SV*1*z*
24	*c*	1	* $I2_13$ *c*	2_12_1.. $P_2Y^*1xxx3yz$

200 $Pm\bar{3}$

1	*a*	$m\bar{3}$.	$Pm\bar{3}m$ *a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	*mmm*..	$Pm\bar{3}m$ *c*	*J*
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	*mm*2..	$Pm\bar{3}m$ *e*	*P*6*z*
6	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*f*	*mm*2..	* $Pm\bar{3}$ *f*	.3. *J*2*x*
6	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
8	*i*	.3.	$Pm\bar{3}m$ *g*	*P*8*xxx*
12	*j*	*m*..	* $Pm\bar{3}$ *j*	*P*6*z*2*x*
12	*k*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*2*x*
24	*l*	1	* $Pm\bar{3}$ *l*	*P*6*z*2*x*2*y*

201 $Pn\bar{3}$

2	*a*	23.	$Im\bar{3}m$ *a*	*I*
4	*b*	.$\bar{3}$.	$Fm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	222..	$Im\bar{3}m$ *b*	J^*
8	*e*	.3.	$Pn\bar{3}m$ *e*	..2 *I*4*xxx*
12	*f*	2..	$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	2..	$Im\bar{3}$ *e*	.3. J^*2x
24	*h*	1	* $Pn\bar{3}$ *h*	*n*.. *I*6*z*2*xy*

202 $Fm\bar{3}$

4	*a*	$m\bar{3}$.	$Fm\bar{3}m$ *a*	*F*
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	23.	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	2/*m*..	$Pm\bar{3}m$ *c*	J_2
24	*e*	*mm*2..	$Fm\bar{3}m$ *e*	*F*6*z*
32	*f*	.3.	$Fm\bar{3}m$ *f*	*F*8*xxx*
48	*g*	2..	$Pm\bar{3}m$ *e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_26z
48	*h*	*m*..	* $Fm\bar{3}$ *h*	*F*6*z*2*x*
96	*i*	1	* $Fm\bar{3}$ *i*	*F*6*z*2*x*2*y*

203 $Fd\bar{3}$

8	*a*	23.	$Fd\bar{3}m$ *a*	*D*
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	.$\bar{3}$.	$Fd\bar{3}m$ *c*	*T*
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	.3.	$Fd\bar{3}m$ *e*	..2 *D*4*xxx*
48	*f*	2..	$Fd\bar{3}m$ *f*	*D*6*z*
96	*g*	1	* $Fd\bar{3}$ *g*	*d*.. *D*6*z*2*xy*

204 $Im\bar{3}$

2	*a*	$m\bar{3}$.	$Im\bar{3}m$ *a*	*I*
6	*b*	*mmm*..	$Im\bar{3}m$ *b*	J^*
8	*c*	.$\bar{3}$.	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	*mm*2..	$Im\bar{3}m$ *e*	*I*6*z*
12	*e*	*mm*2..	* $Im\bar{3}$ *e*	.3. J^*2x
16	*f*	.3.	$Im\bar{3}m$ *f*	*I*8*xxx*
24	*g*	*m*..	* $Im\bar{3}$ *g*	*I*6*z*2*x*
48	*h*	1	* $Im\bar{3}$ *h*	*I*6*z*2*x*2*y*

205 $Pa\bar{3}$

4	*a*	.$\bar{3}$.	$Fm\bar{3}m$ *a*	*F*
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	.3.	* $Pa\bar{3}$ *c*	*bc*.. *F*2*xxx*
24	*d*	1	* $Pa\bar{3}$ *d*	*bc*.. *F*6*xyz*

206 $Ia\bar{3}$

8	*a*	.$\bar{3}$.	$Pm\bar{3}m$ *a*	P_2
8	*b*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
16	*c*	.3.	* $Ia\bar{3}$ *c*	22.. P_22xxx
24	*d*	2..	* $Ia\bar{3}$ *d*	.$\bar{3}$. $J_2S^*V^*1x$
48	*e*	1	* $Ia\bar{3}$ *e*	22.. P_26xyz

207 *P*432

1	*a*	432	$Pm\bar{3}m$ *a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	42.2	$Pm\bar{3}m$ *c*	*J*
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*

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

6	*e*	4..	$Pm\bar{3}m\ e$	$P6z$
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
8	*g*	.3.	$Pm\bar{3}m\ g$	$P8xxx$
12	*h*	2..	$Pm\bar{3}m\ h$	.3. $J4x$
12	*i*	..2	$Pm\bar{3}m\ i$	$P12xx$
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P12xx$
24	*k*	1	* $P432\ k$	$P6z4xy$

208 $P4_232$

2	*a*	23.	$Im\bar{3}m\ a$	I
4	*b*	.32	$Fm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*c*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
6	*d*	222..	$Im\bar{3}m\ b$	J^*
6	*e*	2.22	$Pm\bar{3}n\ c$	W
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ W$
8	*g*	.3.	$Pn\bar{3}m\ e$	..2 $I4xxx$
12	*h*	2..	$Im\bar{3}m\ e$	$I6z$
12	*i*	2..	$Pm\bar{3}n\ g$	.3. $W2z$
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. $W2z$
12	*k*	..2	* $P4_232\ k$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4_2..\ F3x\bar{x}$
12	*l*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ 4_2..\ F3x\bar{x}$
24	*m*	1	* $P4_232\ m$	..2 $I6z2xy$

209 $F432$

4	*a*	432	$Fm\bar{3}m\ a$	F
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F$
8	*c*	23.	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
24	*d*	2.22	$Pm\bar{3}m\ c$	J_2
24	*e*	4..	$Fm\bar{3}m\ e$	$F6z$
32	*f*	.3.	$Fm\bar{3}m\ f$	$F8xxx$
48	*g*	..2	$Fm\bar{3}m\ h$	$F12xx$
48	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F12xx$
48	*i*	2..	$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
96	*j*	1	* $F432\ j$	$F6z4xy$

210 $F4_132$

8	*a*	23.	$Fd\bar{3}m\ a$	D
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ D$
16	*c*	.32	$Fd\bar{3}m\ c$	T
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ T$
32	*e*	.3.	$Fd\bar{3}m\ e$	..2 $D4xxx$
48	*f*	2..	$Fd\bar{3}m\ f$	$D6z$
48	*g*	..2	* $F4_132\ g$	22.. $T3x\bar{x}$
96	*h*	1	* $F4_132\ h$	..2 $D6z2xy$

211 $I432$

2	*a*	432	$Im\bar{3}m\ a$	I
6	*b*	42.2	$Im\bar{3}m\ b$	J^*
8	*c*	.32	$Pm\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
12	*d*	2.22	$Im\bar{3}m\ d$	W^*
12	*e*	4..	$Im\bar{3}m\ e$	$I6z$
16	*f*	.3.	$Im\bar{3}m\ f$	$I8xxx$
24	*g*	2..	$Im\bar{3}m\ g$	.3. J^*4x
24	*h*	..2	$Im\bar{3}m\ h$	$I12xx$
24	*i*	..2	* $I432\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 4.. $P_23x\bar{x}$
48	*j*	1	* $I432\ j$	$I6z4xy$

212 $P4_332$

4	*a*	.32	* $P4_332\ a$	^+Y
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ ^+Y$
8	*c*	.3.	* $P4_332\ c$	$4_3..\ ^+Y2xxx$
12	*d*	..2	* $P4_332\ d$	$4_3..\ ^+Y3x\bar{x}$
24	*e*	1	* $P4_332\ e$	$4_3..\ ^+Y3x\bar{x}2yz$

213 $P4_132$

4	*a*	.32	* $P4_332\ a$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ ^-Y$
4	*b*			^-Y
8	*c*	.3.	* $P4_332\ c$	$4_1..\ ^-Y2xxx$
12	*d*	..2	* $P4_332\ d$	$4_1..\ ^-Y3x\bar{x}$
24	*e*	1	* $P4_332\ e$	$4_1..\ ^-Y3x\bar{x}2yz$

214 $I4_132$

8	*a*	.32	* $I4_132\ a$	$^+Y^*$
8	*b*			$^-Y^*$
12	*c*	2.22	* $I4_132\ c$	^+V
12	*d*			^-V
16	*e*	.3.	* $I4_132\ e$	22.. Y^*2xxx
24	*f*	2..	* $I4_132\ f$	.3. $V2z$
24	*h*	..2	* $I4_132\ h$	$4_3..\ ^+Y^*3x\bar{x}$
24	*g*			$4_1..\ ^-Y^*3x\bar{x}$
48	*i*	1	* $I4_132\ i$	22.. $Y^*3x\bar{x}2yz$

215 $P\bar{4}3m$

1	*a*	$\bar{4}3m$	$Pm\bar{3}m\ a$	P
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
3	*c*	$\bar{4}2.m$	$Pm\bar{3}m\ c$	J
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
4	*e*	.3*m*	* $P\bar{4}3m\ e$	$P4xxx$
6	*f*	2.*mm*	$Pm\bar{3}m\ e$	$P6z$
6	*g*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
12	*h*	2..	$Pm\bar{3}m\ h$	.3. $J4x$
12	*i*	..*m*	* $P\bar{4}3m\ i$	$P6z2xx$
24	*j*	1	* $P\bar{4}3m\ j$	$P6z2xx2y$

216 $F\bar{4}3m$

4	*a*	$\bar{4}3m$	$Fm\bar{3}m\ a$	F
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F$
4	*c*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ F$
16	*e*	.3*m*	* $F\bar{4}3m\ e$	$F4xxx$
24	*f*	2.*mm*	$Fm\bar{3}m\ e$	$F6z$
24	*g*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F6z$
48	*h*	..*m*	* $F\bar{4}3m\ h$	$F6z2xx$
96	*i*	1	* $F\bar{4}3m\ i$	$F6z2xx2y$

217 $I\bar{4}3m$

2	*a*	$\bar{4}3m$	$Im\bar{3}m\ a$	I
6	*b*	$\bar{4}2.m$	$Im\bar{3}m\ b$	J^*
8	*c*	.3*m*	* $I\bar{4}3m\ c$	$I4xxx$
12	*d*	$\bar{4}$..	$Im\bar{3}m\ d$	W^*
12	*e*	2.*mm*	$Im\bar{3}m\ e$	$I6z$
24	*f*	2..	$Im\bar{3}m\ g$	.3. J^*4x
24	*g*	..*m*	* $I\bar{4}3m\ g$	$I6z2xx$
48	*h*	1	* $I\bar{4}3m\ h$	$I6z2xx2y$

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

218 $P\bar{4}3n$

2	*a*	23.	$Im\bar{3}m$ *a*	*I*
6	*b*	222..	$Im\bar{3}m$ *b*	J^*
6	*c*	$\bar{4}$..	$Pm\bar{3}n$ *c*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *W*
6	*d*			*W*
8	*e*	.3.	$I\bar{4}3m$ *c*	*I*4*xxx*
12	*f*	2..	$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	2..	$Pm\bar{3}n$ *g*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *W*2*z*
12	*h*			.3. *W*2*z*
24	*i*	1	* $P\bar{4}3n$ *i*	..*c* *I*6*z*2*xy*

219 $F\bar{4}3c$

8	*a*	23.	$Pm\bar{3}m$ *a*	P_2
8	*b*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*c*	$\bar{4}$..	$Pm\bar{3}m$ *c*	J_2
24	*d*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ J_2
32	*e*	.3.	$P\bar{4}3m$ *e*	$P_2$4*xxx*
48	*f*	2..	$Pm\bar{3}m$ *e*	$P_2$6*z*
48	*g*			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6*z*
96	*h*	1	* $F\bar{4}3c$ *h*	..*n* $P_2$6*z*2*xy*

220 $I\bar{4}3d$

12	*a*	$\bar{4}$..	* $I\bar{4}3d$ *a*	*S*
12	*b*			′*S*
16	*c*	.3.	* $I\bar{4}3d$ *c*	$\bar{4}$.. I_2Y^{**}1*xxx*
24	*d*	2..	* $I\bar{4}3d$ *d*	.3. *S*2*z*
48	*e*	1	* $I\bar{4}3d$ *e*	.3*d* *S*4*xyz*

221 $Pm\bar{3}m$

1	*a*	$m\bar{3}m$	* $Pm\bar{3}m$ *a*	*P*
1	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	4/*mm*.*m*	* $Pm\bar{3}m$ *c*	*J*
3	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	4*m*.*m*	* $Pm\bar{3}m$ *e*	*P*6*z*
6	*f*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
8	*g*	.3*m*	* $Pm\bar{3}m$ *g*	*P*8*xxx*
12	*h*	*mm*2..	* $Pm\bar{3}m$ *h*	.3. *J*4*x*
12	*i*	*m*.*m*2	* $Pm\bar{3}m$ *i*	*P*12*xx*
12	*j*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*12*xx*
24	*k*	*m*..	* $Pm\bar{3}m$ *k*	*P*6*z*4*x*
24	*l*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*4*x*
24	*m*	..*m*	* $Pm\bar{3}m$ *m*	*P*6*z*4*xx*
48	*n*	1	* $Pm\bar{3}m$ *n*	*P*6*z*4*x*2*y*

222 $Pn\bar{3}n$

2	*a*	432	$Im\bar{3}m$ *a*	*I*
6	*b*	42.2	$Im\bar{3}m$ *b*	J^*
8	*c*	.$\bar{3}$.	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	$\bar{4}$..	$Im\bar{3}m$ *d*	W^*
12	*e*	4..	$Im\bar{3}m$ *e*	*I*6*z*
16	*f*	.3.	$Im\bar{3}m$ *f*	*I*8*xxx*
24	*g*	2..	$Im\bar{3}m$ *g*	.3. J^*4*x*
24	*h*	..2	$Im\bar{3}m$ *h*	*I*12*xx*
48	*i*	1	* $Pn\bar{3}n$ *i*	*n*.. *I*6*z*4*xy*

223 $Pm\bar{3}n$

2	*a*	$m\bar{3}$.	$Im\bar{3}m$ *a*	*I*
6	*b*	*mmm*..	$Im\bar{3}m$ *b*	J^*
6	*c*	$\bar{4}$*m*.2	* $Pm\bar{3}n$ *c*	*W*
6	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *W*
8	*e*	.32	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*f*	*mm*2..	$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	*mm*2..	* $Pm\bar{3}n$ *g*	.3. *W*2*z*
12	*h*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *W*2*z*
16	*i*	.3.	$Im\bar{3}m$ *f*	*I*8*xxx*
24	*j*	..2	* $Pm\bar{3}n$ *j*	.3. *W*4*xx*
24	*k*	*m*..	* $Pm\bar{3}n$ *k*	..2 *I*6*z*2*x*
48	*l*	1	* $Pm\bar{3}n$ *l*	..2 *I*6*z*2*x*2*y*

224 $Pn\bar{3}m$

2	*a*	$\bar{4}3m$	$Im\bar{3}m$ *a*	*I*
4	*b*	.$\bar{3}$*m*	$Fm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	$\bar{4}$2.*m*	$Im\bar{3}m$ *b*	J^*
8	*e*	.3*m*	* $Pn\bar{3}m$ *e*	..2 *I*4*xxx*
12	*f*	2.22	$Im\bar{3}m$ *d*	W^*
12	*g*	2.*mm*	$Im\bar{3}m$ *e*	*I*6*z*
24	*h*	2..	$Im\bar{3}m$ *g*	.3. J^*4*x*
24	*i*	..2	* $Pn\bar{3}m$ *i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $\bar{4}$.. *F*6$x\bar{x}$
24	*j*			$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ $\bar{4}$.. *F*6$x\bar{x}$
24	*k*	..*m*	* $Pn\bar{3}m$ *k*	..2 *I*6*z*2*xx*
48	*l*	1	* $Pn\bar{3}m$ *l*	..2 *I*6*z*2*xx*2*y*

225 $Fm\bar{3}m$

4	*a*	$m\bar{3}m$	* $Fm\bar{3}m$ *a*	*F*
4	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	$\bar{4}3m$	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	*m*.*mm*	$Pm\bar{3}m$ *c*	J_2
24	*e*	4*m*.*m*	* $Fm\bar{3}m$ *e*	*F*6*z*
32	*f*	.3*m*	* $Fm\bar{3}m$ *f*	*F*8*xxx*
48	*g*	2.*mm*	$Pm\bar{3}m$ *e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6*z*
48	*h*	*m*.*m*2	* $Fm\bar{3}m$ *h*	*F*12*xx*
48	*i*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*12*xx*
96	*j*	*m*..	* $Fm\bar{3}m$ *j*	*F*6*z*4*x*
96	*k*	..*m*	* $Fm\bar{3}m$ *k*	*F*6*z*4*xx*
192	*l*	1	* $Fm\bar{3}m$ *l*	*F*6*z*4*x*2*y*

226 $Fm\bar{3}c$

8	*a*	432	$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*b*	$m\bar{3}$.	$Pm\bar{3}m$ *a*	P_2
24	*c*	$\bar{4}$*m*.2	$Pm\bar{3}m$ *c*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ J_2
24	*d*	4/*m*..	$Pm\bar{3}m$ *c*	J_2
48	*e*	*mm*2..	$Pm\bar{3}m$ *e*	$P_2$6*z*
48	*f*	4..	$Pm\bar{3}m$ *e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6*z*
64	*g*	.3.	$Pm\bar{3}m$ *g*	$P_2$8*xxx*
96	*h*	..2	$Pm\bar{3}m$ *i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$12*xx*
96	*i*	*m*..	* $Fm\bar{3}c$ *i*	..2 $P_2$6*z*2*x*
192	*j*	1	* $Fm\bar{3}c$ *j*	..2 $P_2$6*z*2*x*2*y*

227 $Fd\bar{3}m$

8	*a*	$\bar{4}3m$	* $Fd\bar{3}m$ *a*	*D*
8	*b*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	.$\bar{3}$*m*	* $Fd\bar{3}m$ *c*	*T*
16	*d*			$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	.3*m*	* $Fd\bar{3}m$ *e*	..2 *D*4*xxx*
48	*f*	2.*mm*	* $Fd\bar{3}m$ *f*	*D*6*z*

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*	$(..2\ I4xxx)_2$
96	*f*	2..	$Im\bar{3}m$ *e*	$I_2 6z$
96	*g*	..2	* $Fd\bar{3}c$ *g*	$\frac{1}{8}\frac{1}{8}\frac{1}{8}\ \bar{4}2..\ F_2 3x\bar{x}$
192	*h*	1	* $Fd\bar{3}c$ *h*	$d.2\ I_2 6z2xy$
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^*4x
24	*h*	*m*.*m*2	* $Im\bar{3}m$ *h*	*I*12*xx*
48	*i*	..2	* $Im\bar{3}m$ *i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4..\ P_2 6x\bar{x}$
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*	$\bar{4}..\ Y^{**}2xxx$
48	*f*	2..	* $Ia\bar{3}d$ *f*	$.3.\ S^*2z$
48	*g*	..2	* $Ia\bar{3}d$ *g*	$\bar{4}a..\ Y^{**}3x\bar{x}$
96	*h*	1	* $Ia\bar{3}d$ *h*	$\bar{4}a..\ I_2 6xyz$

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.

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.

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*
^vD	*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*
^vT	*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*

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* 4*k* $\frac{1}{4}yz$), 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* 8*h* $0yz$ 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 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

14.1

Burzlaff, H., Fischer, W. & Hellner, E. (1968). *Die Gitterkomplexe der Ebenengruppen. Acta Cryst.* A**24**, 57–67.

Fischer, W. & Koch, E. (1974). *Eine Definition des Begriffs 'Gitterkomplex'. Z. Kristallogr.* **139**, 268–278.

Hermann, C. (1935). *Gitterkomplexe/Lattice complexes/Complexes réticulaires.* In *Internationale Tabellen zur Bestimmung von Kristallstrukturen*. 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Reprint with corrections: Ann Arbor: Edwards (1944).]

Koch, E. & Fischer, W. (1978). *Complexes for crystallographic point groups, rod groups and layer groups. Z. Kristallogr.* **147**, 21–38.

Koch, E. & Fischer, W. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion. Acta Cryst.* A**41**, 421–426.

Niggli, P. (1919). *Geometrische Kristallographie des Diskontinuums.* Leipzig: Borntraeger. [Reprint: Wiesbaden: Saendig (1973).]

Zimmermann, H. & Burzlaff, H. (1974). *Zur Definition des Punktlagen- und Gitterkomplex-Begriffs. Z. Kristallogr.* **139**, 252–267.

14.2

Burzlaff, H., Fischer, W. & Hellner, E. (1968). *Die Gitterkomplexe der Ebenengruppen. Acta Cryst.* A**24**, 57–67.

Donnay, J. D. H., Hellner, E. & Niggli, A. (1966). *Symbolism for lattice complexes, revised by a Kiel symposium. Z. Kristallogr.* **123**, 255–262.

Engel, P., Matsumoto, T., Steinmann, G. & Wondratschek, H. (1984). *The non-characteristic orbits of the space groups. Z. Kristallogr.* Supplement issue No. 1.

Fischer, W., Burzlaff, H., Hellner, E. & Donnay, J. D. H. (1973). *Space groups and lattice complexes. NBS Monograph* No. 134. Washington: National Bureau of Standards.

Fischer, W. & Koch, E. (1974). *Eine Definition des Begriffs 'Gitterkomplex'. Z Kristallogr.* **139**, 268–278.

Fischer, W. & Koch, E. (1978). *Limiting forms and comprehensive complexes for crystallographic point groups, rod groups and layer groups. Z. Kristallogr.* **147**, 255–273.

Hermann, C. (1935). *Gitterkomplexe/Lattice complexes/Complexes réticulaires*. In *Internationale Tabellen zur Bestimmung von Kristallstrukturen*. 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Reprint with corrections: Ann Arbor: Edwards (1944).]

Hermann, C. (1960). *Zur Nomenklatur der Gitterkomplexe. Z. Kristallogr.* **113**, 142–154.

Koch, E. (1974). *Die Grenzformen der kubischen Gitterkomplexe. Z. Kristallogr.* **140**, 75–86.

Koch, E. & Fischer, W. (1975). *Automorphismengruppen von Raumgruppen und die Zuordnung von Punktlagen zu Konfigurationslagen. Acta Cryst.* A**31**, 88–95.

Koch, E. & Fischer, W. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion. Acta Cryst.* A**41**, 421–426.

Lawrenson, J. E. & Wondratschek, H. (1976). *The extraordinary orbits of the 17 plane groups. Z. Kristallogr.* **143**, 471–484.

Weissenberg, K. (1925). *Der Aufbau der Kristalle. I. Mitteilung. Die Systematik der Symmetriegruppen von Punktlagen im Diskontinuum. Z. Kristallogr.* **62**, 13–51.

14.3

Baenziger, N. C., Rundle, R. E., Snow, A. T. & Wilson, A. S. (1950). *Compounds of uranium with transition metals of the first long period. Acta Cryst.* **3**, 34–40.

Deschizeaux-Cheruy, M. N., Aubert, J. J., Joubert, J. C., Capponi, J. J. & Vincent, H. (1982). *Relation entre structure et conductivité ionique basse temperature de Ag_3PO_4. Solid State Ionics*, **7**, 171–176.

Fischer, W. (1973). *Existenzbedingungen homogener Kugelpackungen zu kubischen Gitterkomplexen mit weniger als drei Freiheitsgraden. Z. Kristallogr.* **138**, 129–146.

Fischer, W. (1974). *Existenzbedingungen homogener Kugelpackungen zu kubischen Gitterkomplexen mit drei Freiheitsgraden. Z. Kristallogr.* **140**, 50–74.

Fischer, W. (1991*a*). *Tetragonal sphere packings. I. Lattice complexes with zero or one degree of freedom. Z. Kristallogr.* **194**, 67–85.

Fischer, W. (1991*b*). *Tetragonal sphere packings. II. Lattice complexes with two degrees of freedom. Z. Kristallogr.* **194**, 87–110.

Fischer, W. (1993). *Tetragonal sphere packings. III. Lattice complexes with three degrees of freedom. Z. Kristallogr.* **205**, 9–26.

Fischer, W. & Koch, E. (1974). *Kubische Strukturtypen mit festen Koordinaten. Z. Kristallogr.* **140**, 324–330.

Grünbaum, B. (1983). *Tilings, patterns, fabrics and related topics in discrete geometry. Jber. Dtsch. Math.-Verein.* **85**, 1–32.

Grünbaum, B. & Shephard, G. C. (1981). *A hierarchy of classification methods for patterns. Z. Kristallogr.* **154**, 163–187.

Hellner, E. (1965). *Descriptive symbols for crystal-structure types and homeotypes based on lattice complexes. Acta Cryst.* **19**, 703–712.

Hellner, E. (1976*a*). *Verwandtschaftskriterien von Kristallstrukturtypen. I. Z. Anorg. Allg. Chem.* **421**, 37–40.

Hellner, E. (1976*b*). *Verwandtschaftskriterien von Kristallstrukturtypen. II. Die Einführung der Gitterkomplexe P, J und F. Z. Anorg. Allg. Chem.* **421**, 41–48.

Hellner, E. (1976*c*). *Verwandtschaftskriterien von Kristallstrukturtypen. III. Die kubischen Überstrukturen des ReO_3-, Perowskit- und CaF_2-Typs. Z. Anorg. Allg. Chem.* **421**, 49–60.

Hellner, E. (1977). *Verwandtschaftskriterien von Kristallstrukturtypen. IV. Ableitung von Strukturtypen der I-, P- und F-Familien. Z. Anorg. Allg. Chem.* **437**, 60–72.

Hellner, E. (1979). *The frameworks (Bauverbände) of the cubic structure types. Struct. Bonding (Berlin),* **37**, 61–140.

Hellner, E., Koch, E. & Reinhardt, A. (1981). *The homogeneous frameworks of the cubic crystal structures. Phys. Daten-Phys. Data,* **16-2**, 1–67.

Hellner, E. & Sowa, H. (1985). *The cubic structure types described in their space groups with the aid of frameworks. Phys. Daten-Phys. Data,* **16-3**, 1–141.

Hobbie, K. & Hoppe, R. (1986). *Über Oxorhodate der Alkalimetalle: β-$LiRhO_2$. Z. Anorg. Allg. Chem.* **535**, 20–30.

Johnson, C. K., Burnett, M. N. & Dunbar, W. D. (2001). *Crystallographic topology and its applications. Crystallographic Computing 7. Proceedings from the Macromolecular Crystallography Computing School*, edited by P. E. Bourne & K. Watenpaugh. IUCr/Oxford University Press. In the press.

Koch, E. (1973). *Wirkungsbereichspolyeder und Wirkungsbereichsteilungen zu kubischen Gitterkomplexen mit weniger als drei Freiheitsgraden. Z. Kristallogr.* **138**, 196–215.

Koch, E. (1984). *A geometrical classification of cubic point configurations. Z. Kristallogr.* **166**, 23–52.

Koch, E. & Fischer, W. (1978). *Types of sphere packings for crystallographic point groups, rod groups and layer groups. Z. Kristallogr.* **148**, 107–152.

Koch, E. & Hellner, E. (1971). *Die Pattersonkomplexe der Gitterkomplexe. Z. Kristallogr.* **133**, 242–259.

Loeb, A. L. (1970). *A systematic survey of cubic crystal structures. J. Solid State Chem.* **1**, 237–267.

Morss, L. R. (1974). *Crystal structure of dipotassium sodium fluoroaluminate (elpasolite). J. Inorg. Nucl. Chem.* **36**, 3876–3878.

Naor, P. (1958). *Linear dependence of lattice sums. Z. Kristallogr.* **110**, 112–126.