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3.4. Lattice complexes

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3.4.1. The concept of lattice complexes and limiting complexes

3.4.1.1. Introduction

The term *lattice complex* (*Gitterkomplex*) was originally coined by P. Niggli (1919), but he used the term in an ambiguous manner. Later, Hermann (1935) modified and specified the concept of lattice complexes. The rigorous definition used in this chapter was proposed later still by Fischer & Koch (1974*a*) [*cf.* also Koch & Fischer (1978*a*)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at around the same time.

In crystal structures belonging to different structure types and showing different space-group symmetries, some of the atoms may have the same relative locations (*e.g.* Cl in CsCl and F in CaF_2). The concept of *lattice complexes* can be used to reveal relationships between such crystal structures even if their space groups belong to different types.

The terms 'point configuration' (Fischer & Koch, 1974*a*) and 'crystallographic orbit' (Matsumoto & Wondratschek, 1979) have frequently been used as synonyms for sets of points in three-dimensional space $\mathbb{E}^3$ that are equivalent with respect to a space group $\mathcal{G}$. Such sets of points may be classified in two different ways: (1) according to the concept of lattice complexes (German: *Gitterkomplexe*) and of limiting complexes, which goes back to Hermann (1935) and has been defined more strictly by Fischer & Koch (1974*a*); (2) according to the concept of types of crystallographic orbits and of non-characteristic orbits introduced by Wondratschek (1976). As the two approaches[1] are strongly related but not identical, the classes originating from the two concepts will be compared and the differences worked out.

Both terms, 'point configuration' and 'crystallographic orbit', have been used with two slightly different meanings: (1) for sets of points that are equivalent with respect to a given space group, *i.e.* in the mathematical sense of 'orbit'; (2) for such sets of points, but detached from their generating space groups. The second meaning is referred to, for example, if one speaks only of a primitive cubic point lattice. As within both concepts both meanings are required, one has to distinguish between them. In the following, therefore, the term 'crystallographic orbit' is restricted to the first meaning and the term 'point configuration' is restricted to the second meaning.

3.4.1.2. Crystallographic orbits, Wyckoff positions, Wyckoff sets and types of Wyckoff set

In mathematics, an orbit is a very general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group (*cf.* Section 1.1.7). In fact, orbits are always present in crystallography where equivalence classes are defined by means of a group action (*e.g.* a space-group type is the orbit of a space group in the set of all space groups under the action of the affine group). In the present context, however, the term (crystallographic) orbit will be used in a much more restricted sense, as proposed by Wondratschek (1976):

From any point of $\mathbb{E}^3$, the symmetry operations of a given space group $\mathcal{G}$ generate an infinite set of symmetry-equivalent points, called a *crystallographic orbit with respect to* $\mathcal{G}$ or, for short, a *crystallographic orbit* (*cf.* Section 1.4.4). The space group $\mathcal{G}$ is called the *generating space group* of the orbit.

Each point of a crystallographic orbit defines uniquely a largest finite subgroup of $\mathcal{G}$, which maps that point onto itself, its *site-symmetry group* (*cf.* Section 1.4.4). Site-symmetry groups that belong to different points out of the same crystallographic orbit are conjugate subgroups of $\mathcal{G}$.

Example

The points $x, 0, 0$ and $-x+\frac{1}{2}, 0, \frac{1}{2}$; $-x, 0, 0$ and $x+\frac{1}{2}, 0, \frac{1}{2}$ form an orbit of a given space group *Pmna* together with the infinitely many other points that can be generated from the first four by the translations of *Pmna*. The site-symmetry group 2.. of each such point consists of the identity operation 1 and of a twofold rotation. The position of the twofold axis can easily be read from the corresponding coordinate triplet. The site-symmetry groups of the first two points are $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$, respectively. They can be mapped onto another by conjugation *e.g.* with the glide reflection $a\ x, y, \frac{1}{4}$ of *Pmna*. This glide reflection also interchanges the two twofold axes as can easily be learned by inspecting the space-group diagram.

The crystallographic orbits of a given space group $\mathcal{G}$ subdivide the set of all points of $\mathbb{E}^3$ into equivalence classes. It is also possible, however, to define equivalence of orbits on the set of all crystallographic orbits of $\mathcal{G}$:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same Wyckoff position (*cf.* Section 1.4.4) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of $\mathcal{G}$.[2]

Example

The points 0.2, 0, 0 and 0.1, 0, 0.5 belong to different orbits of a given space group *Pmna*. Their site-symmetry groups $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$ are conjugate subgroups of *Pmna* (*cf.* the previous example). Therefore, the two orbits belong to the same Wyckoff position of *Pmna*, namely to 4*e*.

The following definition results in a coarser classification of crystallographic orbits:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same *Wyckoff set* (German: *Konfigurationslage*, *cf.* Fischer & Koch, 1974*a*) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of the affine normalizer of $\mathcal{G}$ (*cf.* Section 1.4.4.3).[3]

[1] The following articles are also related to these topics: Engel (1983); Engel *et al.* (1984); Fischer *et al.* (1973); Fischer & Koch (1978, 1983); Koch (1974); Koch & Fischer (1975, 1978*a*, 1985); Steinmann (1984); Wondratschek (1980).

[2] Instead of conjugation by symmetry operations of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used inner automorphisms of $\mathcal{G}$.

[3] Instead of conjugation by elements of the affine normalizer of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used automorphisms of $\mathcal{G}$.

Accordingly, all orbits of a certain Wyckoff position belong to the same Wyckoff set. The assignment of orbits to Wyckoff sets, therefore, also defines an equivalence relation on the Wyckoff positions of a space group. The Wyckoff sets of the space groups were first tabulated by Koch & Fischer (1975).

Example

In space group *Pmna*, the site-symmetry groups of the points 0.2, 0, 0 and 0.2, 0.5, 0 are {1; 2 *x*, 0, 0} and {1; 2 *x*, $\frac{1}{2}$, 0}. There is no symmetry operation from *Pmna* that maps these site-symmetry groups onto another by conjugation and hence the two corresponding orbits do not belong to the same Wyckoff position of *Pmna*. The Euclidian (and affine) normalizer of *Pmna* is a space group of type *Pmmm* with half the lattice parameters compared with those of *Pmna* (*cf.* Chapter 3.5). It contains *e.g.* the twofold rotation 2 *x*, $\frac{1}{4}$, 0 that maps by conjugation the two site-symmetry groups onto another and also the two axes in the space-group diagram. Therefore, the two orbits belong to the same Wyckoff set even though they belong to the different Wyckoff positions 4*e* and 4*f*.

In analogy to the transition from a single space group to its type, it seems desirable to transfer also the terms 'Wyckoff position' and 'Wyckoff set' to the whole space-group type. For Wyckoff positions, however, such a generalization is not possible: two space groups of the same type can be mapped onto each other by infinitely many isomorphisms or affine mappings. Each isomorphism results in a unique relation between the Wyckoff positions of the two groups, but different isomorphisms may give rise to different relations so that the Wyckoff positions of the same Wyckoff set change their roles.

Such ambiguities, however, cannot occur for Wyckoff sets, because all Wyckoff sets of a certain space group differ in their group-theoretical relations to that group. Therefore, Wyckoff sets may be classified as follows:

Two Wyckoff sets stemming from space groups of the same type belong to the same *type of Wyckoff set* if and only if they are related by an isomorphism (affine mapping) of the two space groups (German: *Klasse von Konfigurationslagen*, *cf.* Fischer & Koch, 1974*a*; Koch & Fischer, 1975). The 219 types of space group in $\mathbb{E}^3$ give rise to 1128 types of Wyckoff set.

Example

Take, in a particular space group of type *P*4/*mmm*, the Wyckoff position 4*l* *x*, 0, 0. The points of each corresponding orbit form squares that replace the points of the tetragonal primitive point lattice of Wyckoff position 1*a*. For all conceivable orbits of 4*l*, the squares have the same orientation, but their edges differ in their lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the orbits of the Wyckoff positions 4*m*, 4*n* and 4*o*, respectively, in the same space group. The four Wyckoff positions 4*l* to 4*o*, all with site symmetry *m*2*m*., make up a Wyckoff set (*cf.* Table 3.4.3.3). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type *P*4/*mmm* is mapped onto another space group of the same type, the Wyckoff set 4*l* to 4*o* as a whole is transformed to 4*l* to 4*o*. The individual Wyckoff positions may be interchanged, however, because of the different possible choices for the origin in each individual space group of type *P*4/*mmm*. All the Wyckoff sets 4*l* to 4*o* stemming from all different space groups of type *P*4/*mmm* constitute together a type of Wyckoff set.

3.4.1.3. Point configurations and lattice complexes, reference symbols

For the comparison of crystal structures belonging to different types, another kind of equivalence relationship between crystallographic orbits may be useful:

One may consider the set of points belonging to a certain orbit without paying attention to the generating space group of the orbit. Such a bare set of points is called a *point configuration*. Two crystallographic orbits are called *configuration equivalent* if their point configurations are identical.

This definition uniquely assigns orbits to point configurations, but not *vice versa*.

Example

Let us consider a certain space group of type $Pm\bar{3}m$ with lattice vectors **a**, **b**, **c** together with two of its non-maximal subgroups, namely $Fm\bar{3}$ with index 4 and *P*432 with index 16, both with lattice vectors 2**a**, 2**b**, 2**c**. The orbit of $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ belongs to Wyckoff position 1*b* of $Pm\bar{3}m$ (site symmetry $m\bar{3}m$), and the corresponding set of points, its point configuration, forms a primitive cubic point lattice. As both subgroups have doubled unit-cell edges, the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ turns to $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. The respective orbits belong to Wyckoff position 8*c* of $Fm\bar{3}$ (site symmetry 23.) and to 8*g* of *P*432 (site symmetry .3.), and both correspond to the original point configuration. Therefore, the three orbits $Pm\bar{3}m$ 1*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, $Fm\bar{3}$ 8*c* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and *P*432 8*g* *x*, *x*, *x* with $x = \frac{1}{4}$ are configuration equivalent (together with several other orbits from certain other subgroups of $Pm\bar{3}m$). They all give rise to one and the same point configuration, a specific primitive cubic lattice of points. The generating space group, however, cannot be identified just by looking at the point configuration.

The *eigensymmetry* of a point configuration is the most comprehensive space group that maps this point configuration onto itself. Accordingly, exactly one crystallographic orbit out of each class of configuration-equivalent orbits stands out because its generating space group coincides with the eigensymmetry of its point configuration. In the case of the example above, this specific orbit is $Pm\bar{3}m$ 1*b* (as long as the origin of $Pm\bar{3}m$ remains unchanged).

The concept of configuration equivalence may also be applied to types of Wyckoff set: two types of Wyckoff set are *configuration equivalent* if and only if for each crystallographic orbit belonging to the first type there exists a configuration-equivalent crystallographic orbit belonging to the second type of Wyckoff set, and *vice versa*. All types of Wyckoff set differ in their crystallographic orbits, but configuration-equivalent types of Wyckoff set result in the same set of point configurations.

A *lattice complex* is the set of all point configurations that correspond to the crystallographic orbits of a certain type of Wyckoff set.

There exist 402 classes of configuration-equivalent types of Wyckoff set and, therefore, 402 lattice complexes in $\mathbb{E}^3$.

Example

Let us consider again the type of Wyckoff set *P*4/*mmm* 4*l* to 4*o* (the last example in Section 3.4.1.2). The set of all corresponding point configurations constitutes a lattice complex. Its point configurations may be derived as described above, but now – instead of starting from just a particular group – starting from all space groups of type $P4/mmm$ with all conceivable positions of the origins and lengths and orientations of the basis vectors. Accordingly, the point configurations may differ in their relative position in space, their orientation, and in the distances between the centres and the size of their squares.

Just as all crystal forms of a particular type may be related to different point-group types, the same lattice complex may occur in different space-group types.

Example

The lattice complex 'cubic primitive lattice' may be generated, among others, in $Pm\bar{3}m$ $1a, b$, in $Fm\bar{3}m$ $8c$ and in $Ia\bar{3}$ $8a, b$ with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ $1a, b$ leads to the same set of point configurations as $Fm\bar{3}m$ $8c$ or $Ia\bar{3}$ $8a, b$. Each point configuration of this lattice complex can be generated by a properly chosen space group of each of these space-group types.

Configuration-equivalent crystallographic orbits do not necessarily belong to configuration-equivalent types of Wyckoff set.

Example

The orbits of the types of Wyckoff set $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$ both refer to the set of all conceivable primitive cubic point lattices. Therefore, these two types of Wyckoff set are configuration equivalent and are associated with the same lattice complex. The type of Wyckoff set $P432$ $8g$ x, x, x, however, comprises apart from crystallographic orbits with $x = \frac{1}{4}$ also those with $x \neq \frac{1}{4}$. The orbits with $x = \frac{1}{4}$ refer to the same set of point configurations as $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, whereas those with $x \neq \frac{1}{4}$ give rise to point configurations with different properties. As a consequence, the type of Wyckoff set $P432$ $8g$ x, x, x is not configuration equivalent with $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, and, therefore, belongs to another lattice complex.

As this example shows, lattice complexes do not form equivalence classes of point configurations, but a certain point configuration may belong to several lattice complexes.

As each type of Wyckoff set uniquely refers to a certain lattice complex, one can also assign all corresponding Wyckoff sets, Wyckoff positions and crystallographic orbits to that lattice complex. A certain lattice complex, however, is frequently related to different types of Wyckoff set.

Among the different types of Wyckoff set belonging to a certain lattice complex, one stands out because its crystallographic orbits show the highest site symmetry. This one is called the *characteristic type of Wyckoff set* of that lattice complex, and the corresponding space-group type its *characteristic space-group type*. All other types of Wyckoff set are referred to as non-characteristic. The term 'characteristic' may also be transferred to particular Wyckoff sets out of the characteristic type. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of its characteristic type.

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

The characteristic space-group type together with the oriented site symmetry expresses the common symmetry properties of all point configurations of a lattice complex and can be used for its identification. For the purpose of *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 arbitrarily chosen, as first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Example

$Pm\bar{3}m$ 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 $1a$ $0, 0, 0$ and $1b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, from which $1a$ has been chosen as the characteristic position. Thus, the reference symbol of this lattice complex is $Pm\bar{3}m$ a.

Example

$Pm\bar{3}m$ is also the characteristic space-group type for a second lattice complex that corresponds to Wyckoff position $8g$ $.3m$ x, x, x. 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.

All types of Wyckoff set (together with their Wyckoff sets and Wyckoff positions) that generate, as described above, the same set of point configurations are assigned to the same lattice complex. Accordingly, the following criterion holds: two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family (*cf.* Section 1.3.4.4). Suitable transformations are translations, proper or improper rotations, isotropic or anisotropic expansions or more general affine mappings (without violation of the metric conditions for the corresponding crystal family), and all their products.

By this criterion, the Wyckoff positions of all space groups (1731 entries in the space-group tables, 1128 types of Wyckoff set) are uniquely assigned to 402 lattice complexes. This assignment was first done by Hermann in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). The corresponding information has also been given by Fischer *et al.* (1973).

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries in the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968). The complexes for the crystallographic subperiodic groups in three-dimensional space, *i.e.* for the crystallographic point groups, rod groups and layer groups, have been derived by Koch & Fischer (1978*a*).

3.4.1.4. Limiting complexes and comprehensive complexes

As has been shown above, lattice complexes define equivalence classes of orbits but not of point configurations. This property gave rise to the concept of limiting complexes and comprehensive complexes (Fischer & Koch, 1974*a*; Koch, 1974).

For morphological crystal forms an almost analogous situation exists. A certain tetragonal prism, for example, may be a general representative of the crystal form 'tetragonal prism' on the one hand or it may be a special representative of the crystal forms 'tetragonal pyramid' or 'tetragonal disphenoid' on the other hand. In the first case the generating point group may belong to the types $4/mmm$, 422, $4/m$ or $\bar{4}2m$ (with site symmetry 2 for each face), in the second case the types of the generating point group are $4mm$ or 4 and $\bar{4}2m$ (site symmetry m) or $\bar{4}$, respectively. The crystal form 'tetragonal prism' is a limiting form of both crystal forms 'tetragonal pyramid' and 'tetragonal disphenoid'.

If a first lattice complex forms a true subset of a second one, *i.e.* if each point configuration of the first lattice complex also belongs to the second one, then the first one is called a *limiting complex* of the second one and the second complex is called a *comprehensive complex* of the first one (*cf.* Koch & Fischer, 1985).

Example

The cubic lattice complex $I\bar{4}3d$ 16c x, x, x involves two limiting complexes, namely $Im\bar{3}m$ 2a 0, 0, 0 and $Ia\bar{3}d$ 16b $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$. The orbits from $I\bar{4}3d$ 16c with $x = 0$ and from $Im\bar{3}m$ 2a are configuration equivalent, and so are the orbits from $I\bar{4}3d$ 16c with $x = \frac{1}{8}$ and from $Ia\bar{3}d$ 16b.

Example

The tetragonal lattice complex $I4_1/amd$ 4a is a comprehensive complex of the cubic complex $Fd\bar{3}m$ 8a. Each orbit of $Fd\bar{3}m$ 8a is configuration equivalent to a crystallographic orbit of a special space group of type $I4_1/amd$ with axial ratio $c/a = (2)^{1/2}$.

Furthermore, two lattice complexes without a limiting-complex relationship may have a non-empty intersection. Then the point configurations of the intersection result in one or, in very exceptional cases, in two or more other lattice complexes (*cf.* Koch, 1974).

Example

The intersection of the two lattice complexes $Im\bar{3}$ 24g and $I\bar{4}3m$ 24g consists of all point configurations belonging to $Im\bar{3}m$ 24h, *i.e.* each point configuration out of this intersection refers to an orbit from $Im\bar{3}m$ 24h 0, x, x and, in addition, to an orbit from $Im\bar{3}$ 24g 0, y, z with $y = z$ and to another one from $I\bar{4}3m$ 24g x, x, z with $z = 0$.

Example

The intersection of the trivariant lattice complexes $Fm\bar{3}c$ 192j and $P432$ 24k consists of two bivariant limiting complexes, namely of $Pm\bar{3}m$ 24k 0, y, z and of $Pm\bar{3}m$ 24m x, x, z.

Each point configuration of a given lattice complex is uniquely related to two space groups: (1) the space group that reflects its eigensymmetry, and (2) a space group that belongs to the characteristic space-group type of the lattice complex under consideration. In most cases the two groups coincide. Only when the point configuration under consideration belongs to a limiting complex is the first group a proper supergroup of the second one.

Complete lists of the limiting complexes of all lattice complexes are not available. Koch (1974) derived the limiting complexes of the cubic lattice complexes. The limiting complexes that refer to specialized coordinate parameters may be derived from a table by Engel *et al.* (1984), who listed the respective non-characteristic orbits for all space-group types. The limiting complexes of the tetragonal and trigonal lattice complexes that are due to metrical specializations are tabulated by Koch & Fischer (2003) and by Koch & Sowa (2005), respectively.

Fischer & Koch (1978) tabulated the limiting complexes for the crystallographic point groups, rod groups and layer groups. As each type of plane group uniquely corresponds to a certain type of isomorphic layer group, information on the limiting complexes of the lattice complexes of the plane groups may easily be extracted from the respective table for the layer groups. This information may also be taken from a list of the non-characteristic orbits of the plane groups by Matsumoto & Wondratschek (1987).

3.4.1.5. Additional properties of lattice complexes

3.4.1.5.1. The degrees of freedom

Each Wyckoff position shows a certain number of coordinate parameters that can be varied independently. For most lattice complexes, this number is the same for any of its Wyckoff positions. For the lattice complex with characteristic Wyckoff position $Pm\bar{3}$ 12j $m..$ 0, y, z, for instance, this number is two. The lattice complex has two degrees of freedom. If, however, the variation of a certain coordinate corresponds to a shift of the point configuration as a whole, the lattice complex has fewer degrees of freedom than the Wyckoff position that is being considered. Therefore, $I4_1$ 8b x, y, z is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8b itself has three coordinate parameters that can be varied independently. The lattice complex $P4/m$ j has two degrees of freedom and refers to Wyckoff positions with two as well as with three independent coordinate parameters, namely to $P4/m$ 4j $m..$ x, y, 0 and to $P4$ 4d 1 x, y, z.

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 can belong 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 ($P4$ d, for example, belongs to the lattice complex with the characteristic Wyckoff position $P4/m$ j).

3.4.1.5.2. 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, orbits where suitably chosen points may be infinitely close together.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm$ 4j $m.2m$ x, x, 0 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. Orbits with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to Wyckoff position $P4/mmm$ 1a.

(ii) The site-symmetry group of every point belonging to the Wyckoff position under consideration is not a proper 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 of Wyckoff position $Pmma$ 2e $\frac{1}{4}$, 0, z. As a consequence, the

Table 3.4.1.1
Reference symbols of the 31 Weissenberg complexes with $f \geq 1$ degrees of freedom in $\mathbb{E}^3$

Weissenberg complex	f	Weissenberg complex	f
$P2_1/m\ e$	2	$I\bar{4}2d\ d$	1
$P2/c\ e$	1	$P4/nmm\ c$	1
$C2/c\ e$	1	$I4_1/acd\ e$	1
$P2_12_12_1\ a$	3	$P3_2\ a$	2
$Pmma\ e$	1	$P3_212\ a$	1
$Pbcm\ d$	2	$P3_221\ a$	1
$Pmmn\ a$	1	$P\bar{3}m1\ d$	1
$Pnma\ c$	2	$P6_1\ a$	2
$Cmcm\ c$	1	$P6_122\ a$	1
$Cmme\ g$	1	$P6_122\ b$	1
$Imma\ e$	1	$P2_13\ a$	1
$P4_3\ a$	2	$I2_13\ a$	1
$P4_322\ a$	1	$I2_13\ b$	1
$P4_322\ c$	1	$Ia\bar{3}\ d$	1
$P4_32_12\ a$	1	$I\bar{4}3d\ c$	1
$I4_122\ f$	1		

distance between any two symmetry-equivalent points belonging to *Pmma e* cannot become shorter than the minimum of $\frac{1}{2}a$, b and c.

A lattice complex refers either to Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are related to Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes without point configurations with infinitesimally short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes were called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. The other 31 Weissenberg complexes with degrees of freedom (24 univariant, 6 bivariant, 1 trivariant) are compiled in Table 3.4.1.1. They have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family (see also Section 3.4.3.1.3).

Example

The Weissenberg complex *Pmma* 2*e* $\frac{1}{4}, 0, z$ is a comprehensive complex of *Pmmm a* and of *Cmmm a*. Within the characteristic Wyckoff position, $\frac{1}{4}, 0, 0$ refers to *Pmmm a* and $\frac{1}{4}, 0, \frac{1}{4}$ to *Cmmm a*.

Apart from the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex *p*2*mg c*.

3.4.2. The concept of characteristic and non-characteristic orbits, comparison with the lattice-complex concept

3.4.2.1. Definitions

The generating space group of any crystallographic orbit may be compared with the eigensymmetry of its point configuration. If both groups coincide, the orbit is called a *characteristic crystallographic orbit*, otherwise it is named a *non-characteristic crystallographic orbit* (Wondratschek, 1976; Engel *et al.*, 1984; see also Section 1.1.7). If the eigensymmetry group contains additional translations in comparison with those of the generating space group, the term *extraordinary orbit* is used (*cf.* also Matsumoto & Wondratschek, 1979). Each class of configuration-equivalent orbits contains exactly one characteristic crystallographic orbit.

The set of all point configurations in $\mathbb{E}^3$ can be divided into 402 equivalence classes by means of their eigensymmetry: two point configurations belong to the same *symmetry type of point configuration* if and only if their characteristic crystallographic orbits belong to the same type of Wyckoff set.

As each crystallographic orbit is uniquely related to a certain point configuration, each equivalence relationship on the set of all point configurations also implies an equivalence relationship on the set of all crystallographic orbits: two crystallographic orbits are assigned to the same *orbit type* (*cf.* also Engel *et al.*, 1984) if and only if the corresponding point configurations belong to the same symmetry type.

In contrast to lattice complexes, neither symmetry types of point configuration nor orbit types can be used to define equivalence relations on Wyckoff positions, Wyckoff sets or types of Wyckoff set. Two crystallographic orbits coming from the same Wyckoff position belong to different orbit types, if – owing to special coordinate values – they differ in the eigensymmetry of their point configurations. Furthermore, two crystallographic orbits with the same coordinate description, but stemming from different space groups of the same type, may belong to different orbit types because of a specialization of the metrical parameters.

Example

The eigensymmetry of orbits from Wyckoff position $P\bar{4}3m$ 4*e* x, x, x with $x = \frac{1}{4}$ or $x = \frac{3}{4}$ is enhanced to $Fm\bar{3}m$ 4*a*, *b* and hence they belong to a different orbit type to those with $x \neq \frac{1}{4}, \frac{3}{4}$.

Example

In general, an orbit belonging to the type of Wyckoff set *I*4/*m* 2*a*, *b* corresponds to a point configuration with eigensymmetry *I*4/*mmm* 2*a*, *b*. If, however, the space group *I*4/*m* has specialized metrical parameters, *e.g.* $c/a = 1$ or $c/a = 2^{1/2}$, then the eigensymmetry of the point configuration is enhanced to $Im\bar{3}m$ 2*a* or $Fm\bar{3}m$ 4*a*, *b*, respectively.

3.4.2.2. Comparison of the concepts of lattice complexes and orbit types

It is the common intention of the lattice-complex and the orbit-type concepts to subdivide the point configurations and crystallographic orbits in $\mathbb{E}^3$ into subsets with certain common properties. With only a few exceptions, the two concepts result in different subsets. As similar but not identical symmetry considerations are used, each lattice complex is uniquely related to a certain symmetry type of point configuration and to a certain orbit type, and *vice versa*. Therefore, the two concepts result in the same number of subsets: there exist 402 lattice complexes and 402 symmetry types of point configuration and orbit types. The differences between the subsets are caused by the different properties of the point configurations and crystallographic orbits used for the classifications (*cf.* also Koch & Fischer, 1985).

The concept of orbit types is entirely based on the eigensymmetry of the particular point configurations: a crystallographic orbit is regarded as an isolated entity, *i.e.* detached from its Wyckoff position and its type of Wyckoff set. On the contrary, lattice complexes result from a hierarchy of classifications of crystallographic orbits into Wyckoff positions, Wyckoff sets, types of Wyckoff set and classes of configuration-equivalent types of

Table 3.4.2.1
Reference symbols of the 28 lattice complexes with $f \geq 1$ degrees of freedom without any limiting complex

Lattice complex	f	Lattice complex	f
$P4/mmm$ l	1	$Pm\bar{3}n$ g	1
$P4_2/mmc$ j	1	$Pm\bar{3}n$ j	1
$I4/mmm$ i	1	$Pn\bar{3}m$ e	1
$P6_222$ g	1	$Pn\bar{3}m$ i	1
$P6/mmm$ l	1	$Fm\bar{3}m$ f	1
$P6/mmm$ p	2	$Fm\bar{3}m$ h	1
$P4_232$ k	1	$Fd\bar{3}m$ g	2
$I432$ i	1	$Im\bar{3}m$ e	1
$I4_132$ h	1	$Im\bar{3}m$ f	1
$I4_132$ i	3	$Im\bar{3}m$ g	1
$Pm\bar{3}m$ e	1	$Im\bar{3}m$ i	1
$Pm\bar{3}m$ i	1	$Im\bar{3}m$ j	2
$Pm\bar{3}m$ k	2	$Im\bar{3}m$ l	3
$Pm\bar{3}m$ m	2	$Ia\bar{3}d$ e	1

Wyckoff set, *i.e.* a crystallographic orbit is always considered as being embedded in its type of Wyckoff set, and the eigensymmetry of a particular point configuration is disregarded. The differences between the two concepts become clear if limiting complexes are considered.

Forty-nine lattice complexes without any limiting complex exist (*cf.* Table 3.4.2.1). They coincide completely with the corresponding symmetry types of point configurations. As can be extracted from the tables by Engel *et al.* (1984) there exist 15 additional lattice complexes without limiting complexes due to specialized coordinates. For fundamental reasons, no cubic or hexagonal complexes allow any metrical specialization.

Example

The lattice complex $P\bar{1}$ a of all triclinic point lattices includes as limiting complexes the 13 other lattice complexes that refer to Bravais lattices. Hence the crystallographic orbits of $P\bar{1}$ a belong to 14 different orbit types.

Example

The lattice complex $Fddd$ a of all orthorhombic diamond patterns includes as limiting complexes those of the tetragonal and the cubic diamond patterns $I4_1/amd$ a and $Fd\bar{3}m$ a, respectively. The orbits of $Fddd$ a with specialized metric, therefore, belong to the orbit types $I4_1/amd$ a or $Fd\bar{3}m$ a.

353 lattice complexes comprise at least one limiting complex. Each of them includes additional point configurations in comparison to the corresponding symmetry type of point configuration (and orbit type), namely those belonging to the limiting complex.

Example

Lattice complex $Im\bar{3}$ 24g 0, y, z comprises for $y = z$ the limiting complex $Im\bar{3}m$ 24h, and for $y = z = \frac{1}{4}$ the limiting complex $Pm\bar{3}m$ 3c. The corresponding orbits with $y = z$ and $y = z = \frac{1}{4}$ do not belong to orbit type $Im\bar{3}$ 24g.

Example

$P4/mmm$ 8r x, x, z comprises for $z = \frac{1}{4}$ the limiting complex $P4/mmm$ 4j, for $x = \frac{1}{4}$ the limiting complex $P4/mmm$ 2g, for $x = z = \frac{1}{4}$ the limiting complex $P4/mmm$ 1a, for $a = c$ and $x = z$ the limiting complex $Pm\bar{3}m$ 8g, and for $a = c$ and $x = z = \frac{1}{4}$ the limiting complex $Pm\bar{3}m$ 1a. Again, none of the corresponding orbits belong to orbit type $P4/mmm$ 8r.

The comparison of an orbit type with its corresponding lattice complex is more intricate. Again, the concept of limiting complexes and comprehensive complexes elucidates the interrelation.

Let A be a lattice complex with a limiting complex B and a comprehensive complex C. The respective orbit types will also be designated A, B and C (*e.g.* A = $Im\bar{3}m$ 24h 0, x, x; B = $Pm\bar{3}m$ 3c, d 0, $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, 0, 0; C = $Im\bar{3}$ 24g 0, y, z). Then a crystallographic orbit from a Wyckoff position of lattice complex A belongs to orbit type A only if it does not correspond to a point configuration of the limiting complex B (*i.e.* only the crystallographic orbits of $Im\bar{3}m$ 24h with $x \neq \frac{1}{4}$ belong to orbit type $Im\bar{3}m$ 24h). The crystallographic orbits of lattice complex A, however, that do correspond to the limiting complex B belong to orbit type B (*i.e.* all crystallographic orbits from $Im\bar{3}m$ 24h with $x = \frac{1}{4}$ belong to orbit type $Pm\bar{3}m$ 3c, d). On the contrary, those orbits that refer to lattice complex C and that happen to correspond to the limiting complex A of C belong to orbit type A instead of orbit type C. All crystallographic orbits of $Im\bar{3}$ 24g 0, y, z with $y = z$ or $y = z = \frac{1}{4}$ create point configurations of lattice complex $Im\bar{3}$ 24g but belong to orbit type $Im\bar{3}m$ 24h or $Pm\bar{3}m$ 3c, d, respectively.

For the comparison of lattice complexes and orbit types the concept of non-characteristic orbits is less helpful than the concept of limiting complexes. In terms of lattice complexes, there exist two basically different reasons for a crystallographic orbit to be non-characteristic:

(1) The crystallographic orbit under consideration belongs to a non-characteristic type of Wyckoff set of a lattice complex. Then this orbit, together with all other orbits from its type of Wyckoff set, is non-characteristic. A characteristic crystallographic orbit necessarily stems from a characteristic Wyckoff set of a lattice complex.
(2) The crystallographic orbit under consideration stands out with respect to the eigensymmetry of its point configuration compared with the other orbits out of its type of Wyckoff sets, *i.e.* it corresponds to a limiting complex. Then this orbit, together with all other orbits referring to that limiting complex, is non-characteristic.

As a consequence, three kinds of non-characteristic orbits may be distinguished:

(1) those that belong to a non-characteristic Wyckoff set, but do not correspond to a limiting complex, *e.g.* all orbits from $Pm\bar{3}$ 6e to h;
(2) those that belong to a characteristic Wyckoff set, but correspond to a limiting complex, *e.g.* $Pm\bar{3}m$ 8g x, x, x with $x = \frac{1}{4}$ or $P4/mmm$ 1a, b with $a = c$;
(3) those that belong to a non-characteristic Wyckoff set and, in addition, correspond to a limiting complex, *e.g.* $Pm\bar{3}$ 8i x, x, x with $x = \frac{1}{4}$.

As these considerations illustrate, limiting complexes and non-characteristic orbits do not coincide and a statement by Engel (1983) proposing this correspondence, therefore, is not correct.

The concept of lattice complexes and limiting complexes on the one hand and of orbit types and non-characteristic orbits on the other hand are complementary in a certain sense: it is possible to derive all orbit types and all non-characteristic orbits from the complete knowledge of lattice complexes and limiting complexes and *vice versa*.

Engel *et al.* (1984) enumerated for all space-group types those non-characteristic orbits that refer to special coordinates, but they excluded all further ones that are based on specialized metrical parameters of the generating space groups or on the simultaneous specialization of metrical and coordinate parameters. A computer program which enables the determination of non-characteristic orbits is now available (*NONCHAR* on the Bilbao Crystallographic Server at http://www.cryst.ehu.es). Lawrenson & Wondratschek (1976) listed the extraordinary orbits of the plane groups, and Matsumoto & Wondratschek (1987) listed the non-characteristic orbits of the plane groups.

The special, but not exceptional, case in which a non-characteristic orbit is produced only if both the coordinates *and* metric are specialized deserves extra concern. The crystallographic orbits from $R\bar{3}$ $6f$ x, y, z with $x = \frac{1}{4}, y = 0, z = \frac{1}{2}$ or $x = \frac{1}{4}, y = \frac{1}{2}, z = 0$ and with the rhombohedral angle $\alpha = 90°$ may be used as an example. The eigensymmetry of the corresponding point configurations is $Pm\bar{3}n$ $6c$, d (corresponding to the position of the Cr atoms in the crystal structure of Cr_3Si). Accordingly, the lattice complex $R\bar{3}$ f comprises $Pm\bar{3}n$ c as limiting complex. $Pm\bar{3}n$ c shows special integral reflection conditions (hkl: $h + k + l = 2n$ or $h = 2n + 1$, $k = 4n$, $l = 4n + 2$; h, k, l permutable), which of course hold for all orbits of that type, *i.e.* also for the special orbits from $R\bar{3}$ f described above. As geometrical structure factors are independent of metrical parameters, these reflection conditions are even valid for crystallographic orbits from $R\bar{3}$ f with $a \neq 90°$ if the coordinates are restricted to $\frac{1}{4}, 0, \frac{1}{2}$ or to $\frac{1}{4}, \frac{1}{2}, 0$.

In general, the following statement holds: if a lattice complex causes special reflection conditions then exactly these conditions are also valid for any crystallographic orbit that refers to a comprehensive complex of that lattice complex if, in addition, this crystallographic orbit may be described by the same coordinate triplets as an orbit of the lattice complex under consideration.

3.4.3. Descriptive lattice-complex symbols and the assignment of Wyckoff positions to lattice complexes

3.4.3.1. Descriptive symbols

3.4.3.1.1. 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 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 3.4.3.2 and 3.4.3.3 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.[4] The comparatively short descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

[4] Some of the descriptive symbols listed in Table 3.4.3.3 differ slightly from those derived by Fischer *et al.* (1973) and used in editions of *International Tables for Crystallography* Volume A before 2002.

Table 3.4.3.1
Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position

Descriptive symbol	Crystal family	Characteristic Wyckoff position
C	o	$Cmmm$ a
	m	$C2/m$ a
D	c	$Fd\bar{3}m$ a
	o	$Fddd$ a
^{v}D	t	$I4_1/amd$ a
E	h	$P6_3/mmc$ c
F	c	$Fm\bar{3}m$ a
	o	$Fmmm$ a
G	h	$P6/mmm$ c
I	c	$Im\bar{3}m$ a
	t	$I4/mmm$ a
	o	$Immm$ a
J	c	$Pm\bar{3}m$ c
J^*	c	$Im\bar{3}m$ b
M	h	$R\bar{3}m$ e
N	h	$P6/mmm$ f
P	c	$Pm\bar{3}m$ a
	h	$P6/mmm$ a
	t	$P4/mmm$ a
	o	$Pmmm$ a
	m	$P2/m$ a
	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	$Fd\bar{3}m$ c
	o	$Fddd$ c
^{v}T	t	$I4_1/amd$ c
^{+}V	c	$I4_132$ c
V^*	c	$Ia\bar{3}d$ c
W	c	$Pm\bar{3}n$ c
W^*	c	$Im\bar{3}m$ d
^{+}Y	c	$P4_332$ a
$^{+}Y^*$	c	$I4_132$ a
Y^{**}	c	$Ia\bar{3}d$ b

3.4.3.1.2. Invariant lattice complexes

An invariant lattice complex in its characteristic Wyckoff position is represented by a capital letter (sometimes in combination with a superscript). The first column of Table 3.4.3.1 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).

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 non-characteristic 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 F is represented in its characteristic Wyckoff position $Fmmm\ a$ by the coordinate triplets $0,0,0,\ \frac{1}{2},\frac{1}{2},0,\ 0,\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},0,\frac{1}{2}$. In $Pnnn\ e$ (origin choice 1), it is described by $\frac{1}{4},\frac{1}{4},\frac{1}{4},\ \frac{3}{4},\frac{3}{4},\frac{1}{4},\ \frac{1}{4},\frac{3}{4},\frac{3}{4}$ and $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ and, therefore, receives the descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}F$.

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

In non-characteristic Wyckoff positions, the descriptive symbols P and I may be replaced by C and F, respectively (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).

3.4.3.1.3. Lattice complexes with degrees of freedom

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

Example

$0\frac{1}{2}0$ ..2 $C4xxz$ is the descriptive symbol of the lattice complex $P4/nbm\ m$ in its characteristic position: $0\frac{1}{2}0$ is the shift vector, ..2 the distribution symmetry, C the central part and $4xxz$ the site-set symbol.

Normally, the central part is the symbol of an invariant lattice complex. The shift vector and central part together should be interpreted as described in Section 3.4.3.1.2. The point configurations of the Wyckoff position being considered 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 symmetry-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) $I4xxx$ ($I\bar{4}3m\ 8c\ x,x,x$) designates a lattice complex, the point configurations of which are composed of tetrahedra $4xxx$ in parallel orientation replacing the points of a cubic body-centred lattice I. The vertices of these tetrahedra are located on body diagonals.

(2) ..2 $I4xxx$ ($Pn\bar{3}m\ 8e\ x,x,x$) represents the lattice complex for which, in contrast to the first example, the tetrahedra $4xxx$ around $0,0,0$ 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 $P4_2/mcm\ 8l\ x,0,\frac{1}{4}$. Each corresponding point configuration consists of squares of points $4x$ replacing the points of a tetragonal primitive lattice P. In comparison with $P4x$, $00\frac{1}{4}\ P_c4x$ shows a unit-cell enlargement by $\mathbf{c}' = 2\mathbf{c}$ and a subsequent shift by $0,0,\frac{1}{4}$.

In the case of a Weissenberg complex (*cf.* Section 3.4.1.5.2; Weissenberg, 1925; Fischer *et al.*, 1973), the central part of the descriptive symbol always consists of two (or more) symbols of invariant lattice complexes belonging to the same crystal family and forming limiting complexes of the Weissenberg complex under consideration. The shift vector then refers to the first limiting complex. The corresponding site-set symbols are distinguished by containing the number 1 as the only number, *i.e.* each site set consists of only one point.

Example

In $\frac{1}{4}00$ .2. P_aB1z ($Pmma$ $2e$ $\frac{1}{4}, 0, z$), each of the two points $\frac{1}{4}, 0, 0$ and $\frac{3}{4}, 0, 0$, represented by $\frac{1}{4}00$ P_a, is replaced by a site set $1z$ containing only one point, *i.e.* the points of $\frac{1}{4}00$ P_a are shifted along the z axis. The shifts of the two points are related by a twofold rotation .2., *i.e.* are running in opposite directions. The point configurations of the two limiting complexes P_a and B refer to the special parameter values $z = 0$ and $z = \frac{1}{4}$, respectively.

The central parts of some lattice complexes with two or three degrees of freedom are formed by the descriptive symbol of a univariant Weissenberg complex instead of that of an invariant lattice complex. This is the case only if the corresponding characteristic space-group type does not refer to a suitable invariant lattice complex.

Example

In $\frac{1}{4}00$ .2. P_aB1z2y ($Pmma$ $4k$ $\frac{1}{4}, y, z$), each of the two points $\frac{1}{4}, 0, z$ and $\frac{3}{4}, 0, \bar{z}$, represented by $\frac{1}{4}00$ .2. P_aB1z, is replaced by a site set $2y$ of two points forming a dumbbell. These dumbbells are oriented parallel to the y axis.

The symbol of a non-characteristic Wyckoff position is deduced from that of the characteristic position. The four parts of the descriptive symbol are subjected to the transformation necessary to map the characteristic Wyckoff position onto the Wyckoff position under consideration.

Example

The lattice complex with characteristic Wyckoff position $Imma$ $8h$ $0, y, z$ has the descriptive symbol .2. B_b2yz for this position. Another Wyckoff position of this lattice complex is $Imma$ $8i$ $x, \frac{1}{4}, z$. The corresponding point configurations are mapped onto each other by interchanging positive x and negative y directions and shifting by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. Therefore, the descriptive symbol for Wyckoff position $Imma$ i is $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. A_a2xz.

In some cases, the Wyckoff position described by a lattice-complex symbol has more degrees of freedom than the lattice complex (see Section 3.4.1.5.1). In such cases, a letter (or a string of letters) in brackets is added to the symbol.

Examples

$tP[z]$ for $P4$ a, $aP[xyz]$ for $P1$ a.

3.4.3.1.4. *Properties of the descriptive symbols*

Different kinds of relations between lattice complexes are brought out.

Examples

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

In many cases, limiting-complex relations can be deduced from the symbols. This applies to limiting complexes due either to special metrical parameters (*e.g.* $cP \leftrightarrow rP$ *etc.*) or to special values of coordinates (*e.g.* both $P4x$ and $P4xx$ are limiting complexes of $P4xy$). If the site set consists of only one point, the central part of the symbol specifies all corresponding limiting complexes without degrees of freedom that are due to special values of the coordinates (*e.g.* 2_12_1. $FA_aB_bC_cI_aI_bI_c1xyz$ for the general position of $P2_12_12_1$).

3.4.3.2. Assignment of Wyckoff positions to Wyckoff sets and to lattice complexes

In Tables 3.4.3.2 and 3.4.3.3, the Wyckoff positions of all plane and space groups, respectively, are listed. Each Wyckoff position is identified by its Wyckoff letter together with its oriented site-symmetry symbol. It is assigned to its lattice complex by means of the reference symbol (*cf.* Section 3.4.1.3). Characteristic Wyckoff positions are marked by asterisks (*e.g.* $2e$ in $P2/c$). If in a particular space group several Wyckoff positions belong to the same Wyckoff set (*cf.* Sections 1.4.4.3 and 3.4.1.2; Koch & Fischer, 1975), the reference symbol is given only once (*e.g.* Wyckoff positions $4l$ to $4o$ in $P4/mmm$). To enable this, the usual sequence of Wyckoff positions had to be changed in a few cases (*e.g.* in $P4_2/mcm$). For Wyckoff positions assigned to the same lattice complex but belonging to different Wyckoff sets, the reference symbol is repeated. In $I4/m$, for example, Wyckoff positions $4c$ and $4d$ are both assigned to the lattice complex $P4/mmm$ a. They do not belong, however, to the same Wyckoff set because the site-symmetry groups $2/m..$ of $4c$ and $\bar{4}..$ of $4d$ are different.

The last columns of Tables 3.4.3.2 and 3.4.3.3 show the descriptive lattice-complex symbol for each Wyckoff position.

3.4.4. Applications of the lattice-complex concept

3.4.4.1. Geometrical properties of point configurations

To study the geometrical properties of all point configurations in three-dimensional space, it is not necessary to consider all Wyckoff positions of the space groups or all 1128 types of Wyckoff set. Instead, one may restrict the investigations to the characteristic Wyckoff positions of the 402 lattice complexes. The results can then be transferred to all non-characteristic Wyckoff positions of the lattice complexes, as listed in Tables 3.4.3.2 and 3.4.3.3.

The determination of all types of sphere packings with cubic and tetragonal symmetry forms an example for this kind of procedure (Fischer, 1973, 1974, 1991*a*,*b*, 1993). The cubic lattice complex $I4xxx$, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ $8c$ $.3m.$ x, x, x. Sphere packings with three-membered rings and nine contacts per sphere are formed if $x = 3/16$. The parameter region $3/16 < x < \frac{1}{4}$ corresponds to sphere packings with four-membered rings and six contacts per sphere (*cf.* Fischer, 1973). Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (Deschizeaux-Cheruy *et al.*, 1982) and the oxygen atoms occupy Wyckoff position $8e$ $.3.$ x, x, x, which also belongs to lattice complex $I4xxx$. Comparison of the coordinate parameter x = 0.1491 for the oxygen atoms with the sphere-packing parameters listed for $I\bar{4}3m$ c shows directly that the oxygen arrangement in this crystal structure does not form a sphere packing.

Other examples for this approach are the derivation of crystal potentials (Naor, 1958), of coordinate restrictions in

(*continued on page* 823)

Table 3.4.3.2
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 3.4.3.3
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*	$P2xyz$

3 *P*2

1	*a*	2		$P2/m$ *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		$P2/m$ *m*	$P2xz[y]$

4 $P2_1$

2	*a*	1		$P2_1/m$ *e*	2_1 $P_bACI1xz[y]$

5 *C*2

2	*a*	2		$C2/m$ *a*	$C[y]$
2	*b*				$00\frac{1}{2}$ $C[y]$
4	*c*	1		$C2/m$ *i*	$C2xz[y]$

6 *Pm*

1	*a*	*m*		$P2/m$ *a*	$P[xz]$
1	*b*				$0\frac{1}{2}0$ $P[xz]$
2	*c*	1		$P2/m$ *i*	$P2y[xz]$

7 *Pc*

2	*a*	1		$P2/c$ *e*	c $P_cA1y[xz]$

8 *Cm*

2	*a*	*m*		$C2/m$ *a*	$C[xz]$
4	*b*	1		$C2/m$ *g*	$C2y[xz]$

9 *Cc*

4	*a*	1		$C2/c$ *e*	$\bar{1}$ $C_cF1y[xz]$

10 $P2/m$

1	*a*	$2/m$	*	$P2/m$ *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	*	$P2/m$ *i*	$P2y$
2	*j*				$\frac{1}{2}00$ $P2y$
2	*k*				$00\frac{1}{2}$ $P2y$
2	*l*				$\frac{1}{2}0\frac{1}{2}$ $P2y$
2	*m*	*m*	*	$P2/m$ *m*	$P2xz$
2	*n*				$0\frac{1}{2}0$ $P2xz$
4	*o*	1	*	$P2/m$ *o*	$P2xz2y$

11 $P2_1/m$

2	*a*	$\bar{1}$		$P2/m$ *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 $C2/m$

2	*a*	$2/m$	*	$C2/m$ *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*	$\bar{1}$		$P2/m$ *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	*	$C2/m$ *g*	$C2y$
4	*h*				$00\frac{1}{2}$ $C2y$
4	*i*	*m*	*	$C2/m$ *i*	$C2xz$
8	*j*	1	*	$C2/m$ *j*	$C2xz2y$

13 $P2/c$

2	*a*	$\bar{1}$		$P2/m$ *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	*	$P2/c$ *e*	$00\frac{1}{4}$ c P_cA1y
2	*f*				$\frac{1}{2}0\frac{1}{4}$ c P_cA1y
4	*g*	1	*	$P2/c$ *g*	2 P_c2xyz

14 $P2_1/c$

2	*a*	$\bar{1}$		$C2/m$ *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 $A2xyz$

15 $C2/c$

4	*a*	$\bar{1}$		$C2/m$ *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	*	$C2/c$ *e*	$00\frac{1}{4}$ $\bar{1}$ C_cF1y
8	*f*	1	*	$C2/c$ *f*	2_1 C_c2xyz

Table 3.4.3.3 (continued)

16 P222

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				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	i	2..		Pmmm i	$P2x$
2	j				$00\frac{1}{2}\ P2x$
2	k				$0\frac{1}{2}0\ P2x$
2	l				$0\frac{1}{2}\frac{1}{2}\ P2x$
2	m	.2.			$P2y$
2	n				$00\frac{1}{2}\ P2y$
2	o				$\frac{1}{2}00\ P2y$
2	p				$\frac{1}{2}0\frac{1}{2}\ P2y$
2	q	..2			$P2z$
2	r				$\frac{1}{2}00\ P2z$
2	s				$0\frac{1}{2}0\ P2z$
2	t				$\frac{1}{2}\frac{1}{2}0\ P2z$
4	u	1	*	P222 u	$P2x2yz$

17 $P222_1$

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 $P2_12_12$

2	a	..2		Pmmn a	$2_1..\ CI1z$
2	b				$0\frac{1}{2}0\ 2_1..\ CI1z$
4	c	1	*	$P2_12_12\ c$	$2_1..\ CI1z2xy$

19 $P2_12_12_1$

4	a	1	*	$P2_12_12_1\ a$	$2_12_1.\ FA_aB_bC_cI_aI_bI_c1xyz$

20 $C222_1$

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 C222

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	$C2x$
4	f				$00\frac{1}{2}\ C2x$
4	g	.2.			$C2y$
4	h				$00\frac{1}{2}\ C2y$
4	i	..2		Cmmm k	$C2z$
4	j				$0\frac{1}{2}0\ C2z$
4	k	..2		Cmme g	$\frac{1}{4}\frac{1}{4}0\ 2..\ P_{ab}F1z$
8	l	1	*	C222 l	$C2x2yz$

22 F222

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	$F2x$
8	j				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2x$
8	f	.2.			$F2y$
8	i				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2y$
8	g	..2			$F2z$
8	h				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F2z$
16	k	1	*	F222 k	$F2x2yz$

23 I222

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	$I2x$
4	f				$00\frac{1}{2}\ I2x$
4	g	.2.			$I2y$
4	h				$\frac{1}{2}00\ I2y$
4	i	..2			$I2z$
4	j				$0\frac{1}{2}0\ I2z$
8	k	1	*	I222 k	$I2x2yz$

24 $I2_12_12_1$

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 Pmm2

1	a	mm2		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	$P2x[z]$
2	f				$0\frac{1}{2}0\ P2x[z]$
2	g	m..			$P2y[z]$
2	h				$\frac{1}{2}00\ P2y[z]$
4	i	1		Pmmm u	$P2x2y[z]$

26 $Pmc2_1$

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 Pcc2

2	a	..2		Pmmm a	$P_c[z]$
2	b				$0\frac{1}{2}0\ P_c[z]$

Table 3.4.3.3 (continued)

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 *Pca*2$_1$					
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*	$2..\ A2xy[z]$
31 *Pmn*2$_1$					
2	*a*	*m*..		*Pmmn a*	$..2_1\ BI1y[z]$
4	*b*	1		*Pmmn e*	$..2_1\ BI1y2x[z]$
32 *Pba*2					
2	*a*	..2		*Cmmm a*	$C[z]$
2	*b*				$0\frac{1}{2}0\ C[z]$
4	*c*	1		*Pbam g*	$b..\ C2xy[z]$
33 *Pna*2$_1$					
4	*a*	1		*Pnma c*	$\bar{1}2_1.\ C_cA_aFI_a1xy[z]$
34 *Pnn*2					
2	*a*	..2		*Immm a*	$I[z]$
2	*b*				$0\frac{1}{2}0\ I[z]$
4	*c*	1		*Pnnm g*	$n..\ I2xy[z]$
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*	$C2x[z]$
4	*e*	*m*..			$C2y[z]$
8	*f*	1		*Cmmm p*	$C2x2y[z]$
36 *Cmc*2$_1$					
4	*a*	*m*..		*Cmcm c*	$2_1..\ C_cF1y[z]$
8	*b*	1		*Cmcm g*	$2_1..\ C_cF1y2x[z]$
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*	$n..\ C_c2xy[z]$
38 *Amm*2					
2	*a*	*mm*2		*Cmmm a*	$A[z]$
2	*b*				$\frac{1}{2}00\ A[z]$
4	*c*	.*m*.		*Cmmm k*	$A2x[z]$
4	*d*	*m*..		*Cmmm g*	$A2y[z]$
4	*e*				$\frac{1}{2}00\ A2y[z]$
8	*f*	1		*Cmmm n*	$A2x2y[z]$
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*	$0\frac{1}{4}0\ ..2\ P_{bc}F1x[z]$
8	*d*	1		*Cmme m*	$.m.\ P_{bc}2xy[z]$
40 *Ama*2					
4	*a*	..2		*Cmmm a*	$A_a[z]$
4	*b*	*m*..		*Cmcm c*	$\frac{1}{4}00\ ..2_1\ A_aF1y[z]$
8	*c*	1		*Cmcm f*	$.n.\ A_a2xy[z]$
41 *Aea*2					
4	*a*	..2		*Fmmm a*	$F[z]$
8	*b*	1		*Cmce f*	$.2.\ F2xy[z]$
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*	$F2y[z]$
8	*d*	.*m*.			$F2x[z]$
16	*e*	1		*Fmmm m*	$F2x2y[z]$
43 *Fdd*2					
8	*a*	..2		*Fddd a*	$D[z]$
16	*b*	1	*	*Fdd2 b*	$d..\ D2xy[z]$
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*	$I2x[z]$
4	*d*	*m*..			$I2y[z]$
8	*e*	1		*Immm l*	$I2x2y[z]$
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*	$b..\ C_c2xy[z]$
46 *Ima*2					
4	*a*	..2		*Cmmm a*	$A_a[z]$
4	*b*	*m*..		*Imma e*	$\frac{1}{4}00\ 2..\ A_aC_c1y[z]$
8	*c*	1		*Imma h*	$2..\ A_a2xy[z]$
47 *Pmmm*					
1	*a*	*mmm*	*	*Pmmm a*	P
1	*b*				$\frac{1}{2}00\ P$

Table 3.4.3.3 (continued)

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*	*2mm*	*	*Pmmm i*	$P2x$
2	*j*				$00\frac{1}{2}\ P2x$
2	*k*				$0\frac{1}{2}0\ P2x$
2	*l*				$0\frac{1}{2}\frac{1}{2}\ P2x$
2	*m*	*m2m*			$P2y$
2	*n*				$00\frac{1}{2}\ P2y$
2	*o*				$\frac{1}{2}00\ P2y$
2	*p*				$\frac{1}{2}0\frac{1}{2}\ P2y$
2	*q*	*mm2*			$P2z$
2	*r*				$0\frac{1}{2}0\ P2z$
2	*s*				$\frac{1}{2}00\ P2z$
2	*t*				$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*u*	*m..*	*	*Pmmm u*	$P2y2z$
4	*v*				$\frac{1}{2}00\ P2y2z$
4	*w*	*.m.*			$P2x2z$
4	*x*				$0\frac{1}{2}0\ P2x2z$
4	*y*	*..m*			$P2x2y$
4	*z*				$00\frac{1}{2}\ P2x2y$
8	*α*	1	*	*Pmmm α*	$P2x2y2z$
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*	*mm2*	*	*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*	$.2.\ B2yz2x$

Table 3.4.3.3 (continued)

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*	$2.m\ P_{bc}2xyz$
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*	$I2z$
4	*f*				$0\frac{1}{2}0\ I2z$
4	*g*	..*m*	*	*Pnnm g*	$n..\ I2xy$
8	*h*	1	*	*Pnnm h*	$n..\ I2xy2z$
59 *Pmmn*					
2	*a*	*mm*2	*	*Pmmn a*	$2_1..\ CI1z$
2	*b*				$0\frac{1}{2}0\ 2_1..\ CI1z$
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*	$2_1..\ CI1z2y$
4	*f*	.*m*.			$.2_1.\ CI1z2x$
8	*g*	1	*	*Pmmn g*	$\frac{1}{4}\frac{1}{4}0\ mm.\ P_{ab}2xyz$
60 *Pbcn*					
4	*a*	$\bar{1}$		*Cmmm a*	C_c
4	*b*				$0\frac{1}{2}0\ C_c$
4	*c*	.2.		*Cmcm c*	$00\frac{1}{4}\ 2_1..\ C_cF1y$
8	*d*	1	*	*Pbcn d*	$b2.\ C_c2xyz$
61 *Pbca*					
4	*a*	$\bar{1}$		*Fmmm a*	F
4	*b*				$00\frac{1}{2}\ F$
8	*c*	1	*	*Pbca c*	$bc.\ F2xyz$
62 *Pnma*					
4	*a*	$\bar{1}$		*Cmmm a*	B_b
4	*b*				$00\frac{1}{2}\ B_b$
4	*c*	.*m*.	*	*Pnma c*	$0\frac{1}{4}0\ \bar{1}.2_1\ B_bA_aFI_a1xz$
8	*d*	1	*	*Pnma d*	$.ma\ B_b2xyz$
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*	$00\frac{1}{4}\ 2_1..\ C_cF1y$
8	*d*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_2$
8	*e*	2..		*Cmmm g*	C_c2x
8	*f*	*m*..	*	*Cmcm f*	$.n.\ C_c2yz$
8	*g*	..*m*	*	*Cmcm g*	$00\frac{1}{4}\ 2_1..\ C_cF1y2x$
16	*h*	1	*	*Cmcm h*	$.n.\ C_c2yz2x$
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*	$F2x$
8	*e*	.2.		*Pmma e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ (2..\ P_cA1y)_{ab}$
8	*f*	*m*..	*	*Cmce f*	$.2.\ F2yz$
16	*g*	1	*	*Cmce g*	$.2.\ F2yz2x$
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*	$C2x$
4	*h*				$00\frac{1}{2}\ C2x$
4	*i*	*m*2*m*			$C2y$
4	*j*				$00\frac{1}{2}\ C2y$
4	*k*	*mm*2	*	*Cmmm k*	$C2z$
4	*l*				$0\frac{1}{2}0\ C2z$
8	*m*	..2		*Pmmm i*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}2z$
8	*n*	*m*..	*	*Cmmm n*	$C2y2z$
8	*o*	.*m*.			$C2x2z$
8	*p*	..*m*	*	*Cmmm p*	$C2x2y$
8	*q*				$00\frac{1}{2}\ C2x2y$
16	*r*	1	*	*Cmmm r*	$C2x2y2z$

Table 3.4.3.3 (continued)

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*	$00\frac{1}{4}\ C_c2x$
8	*h*	.2.			$00\frac{1}{4}\ C_c2y$
8	*i*	..2		*Cmmm k*	C_c2z
8	*j*				$0\frac{1}{2}0\ C_c2z$
8	*k*	..2		*Fmmm g*	$\frac{1}{4}\frac{1}{4}0\ F2z$
8	*l*	..*m*	*	*Cccm l*	$c..\ C_c2xy$
16	*m*	1	*	*Cccm m*	$c..\ C_c2xy2z$

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*	$0\frac{1}{4}0\ 2..\ P_{ab}F1z$
8	*h*	2..		*Pmmm i*	$P_{ab}2x$
8	*i*				$00\frac{1}{2}\ P_{ab}2x$
8	*j*	.2.			$\frac{1}{4}00\ P_{ab}2y$
8	*k*				$\frac{1}{4}0\frac{1}{2}\ P_{ab}2y$
8	*l*	..2		*Pmmm i*	$\frac{1}{4}00\ P_{ab}2z$
8	*m*	*m*..	*	*Cmme m*	$.m.\ P_{ab}2yz$
8	*n*	.*m*.			$0\frac{1}{4}0\ m..\ P_{ab}2xz$
16	*o*	1	*	*Cmme o*	$.m.\ P_{ab}2yz2x$

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*	$F2x$
8	*f*	.2.			$F2y$
8	*g*	..2		*Fmmm g*	$F2z$
8	*h*	..2		*Cmme g*	$\frac{1}{4}\frac{1}{4}0\ (2..\ P_{ab}F1z)_c$
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*	$F2x$
8	*h*	*m*2*m*			$F2y$
8	*i*	*mm*2			$F2z$
16	*j*	..2		*Pmmm i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22z$
16	*k*	.2.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22y$
16	*l*	2..			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_22x$
16	*m*	*m*..	*	*Fmmm m*	$F2y2z$
16	*n*	.*m*.			$F2x2z$
16	*o*	..*m*			$F2x2y$
32	*p*	1	*	*Fmmm p*	$F2x2y2z$

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*	$D2x$
16	*f*	.2.			$D2y$
16	*g*	..2			$D2z$
32	*h*	1	*	*Fddd h*	$d..\ D2x2yz$

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*	$I2x$
4	*f*				$0\frac{1}{2}0\ I2x$
4	*g*	*m*2*m*			$I2y$
4	*h*				$00\frac{1}{2}\ I2y$
4	*i*	*mm*2			$I2z$
4	*j*				$\frac{1}{2}00\ I2z$
8	*k*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*l*	*m*..	*	*Immm l*	$I2y2z$
8	*m*	.*m*.			$I2x2z$
8	*n*	..*m*			$I2x2y$
16	*o*	1	*	*Immm o*	$I2x2y2z$

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*	$00\frac{1}{4}\ C_c2x$
8	*g*	.2.			$00\frac{1}{4}\ C_c2y$
8	*h*	..2		*Cmmm k*	C_c2z
8	*i*				$0\frac{1}{2}0\ C_c2z$
8	*j*	..*m*	*	*Ibam j*	$c..\ C_c2xy$
16	*k*	1	*	*Ibam k*	$c..\ C_c2xy2z$

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*	$22.\ P_22xyz$

Table 3.4.3.3 (continued)

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*	$0\frac{1}{4}0\ .2.\ B_bA_a1z$
8	*f*	2..		*Cmmm g*	B_b2x
8	*g*	.2.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ A_a2y$
8	*h*	*m*..	*	*Imma h*	$.2.\ B_b2yz$
8	*i*	.*m*.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 2..\ A_a2xz$
16	*j*	1	*	*Imma j*	$.2.\ B_b2yz2x$

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*	$P4xy[z]$

76 $P4_1$

4	*a*	1	*	$P4_3\ a$	$4_1..\ P_{cc}{}^vDI_c1xy[z]$

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		$P4_2/m\ j$	$\bar{4}..\ P_c2xy[z]$

78 $P4_3$

4	*a*		*	$P4_3\ a$	$4_3..\ P_{cc}{}^vDI_c1xy[z]$

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*	$I4xy[z]$

80 $I4_1$

4	*a*	2..		$I4_1/amd\ a$	${}^vD[z]$
8	*b*	1	*	$I4_1\ b$	$4_1..\ {}^vD2xy[z]$

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*	$P2z$
2	*f*				$\frac{1}{2}\frac{1}{2}0\ P2z$
2	*g*	2..		*P*4/*nmm c*	$0\frac{1}{2}0\ ..2\ CI1z$
4	*h*	1	*	$P\bar{4}\ h$	$P4xyz$

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*	$I2z$
4	*f*				$0\frac{1}{2}\frac{1}{4}\ I2z$
8	*g*	1	*	$I\bar{4}\ g$	$I4xyz$

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*	$P2z$
2	*h*				$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*i*	2..		*P*4/*mmm g*	$0\frac{1}{2}0\ C2z$
4	*j*	*m*..	*	*P*4/*m j*	$P4xy$
4	*k*				$00\frac{1}{2}\ P4xy$
8	*l*	1	*	*P*4/*m l*	$P4xy2z$

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*	$0\frac{1}{2}0\ I2z$
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*	$0\frac{1}{2}0\ ..2\ CI1z$
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*	$C2z$
8	*g*	1	*	*P*4/*n g*	$\bar{1}\ C4xyz$

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*	$I2z$
8	*g*	1	*	$P4_2/n\ g$	$n..\ I4xyz$

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*	$0\frac{1}{2}\frac{1}{4}\ C_c$

Table 3.4.3.3 (continued)

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*	$\bar{4}$..		$I4_1/amd\ a$	^vD
4	*b*				$00\frac{1}{2}\ {}^vD$
8	*c*	$\bar{1}$		$I4_1/amd\ c$	^vT
8	*d*				$00\frac{1}{2}\ {}^vT$
8	*e*	2..		$I4_1/amd\ e$	^vD2z
16	*f*	1	*	$I4_1/a\ f$	$a..\ {}^vD4xyz$

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*				$\frac{1}{2}\frac{1}{2}0\ P2z$
4	*i*	2..		*P*4/*mmm g*	$0\frac{1}{2}0\ C2z$
4	*j*	..2		*P*4/*mmm j*	*P*4*xx*
4	*k*				$00\frac{1}{2}\ P4xx$
4	*l*	.2.		*P*4/*mmm l*	*P*4*x*
4	*m*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P4x$
4	*n*				$00\frac{1}{2}\ P4x$
4	*o*				$\frac{1}{2}\frac{1}{2}0\ P4x$
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*	$0\frac{1}{2}0\ ..2\ CI1z$
4	*d*	2..		*P*4/*mmm g*	*C*2*z*
4	*e*	..2		*P*4/*mbm g*	.*b*. *C*2*xx*
4	*f*				$00\frac{1}{2}\ .b.\ C2xx$
8	*g*	1	*	$P42_12\ g$	$.2_1.\ C2xx2yz$

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	*	$P4_322\ c$	$00\frac{3}{8}\ 4_1..\ P_{cc}{}^vD1xx$
8	*d*	1	*	$P4_322\ d$	$00\frac{3}{4}\ 4_1..\ P_{cc}I_c1x2yz$

92 $P4_12_12$

4	*a*	..2	*	$P4_32_12\ a$	$4_1..\ I_c{}^vD1xx$
8	*b*	1	*	$P4_32_12\ b$	$4_1..\ I_c{}^vD1xx2yz$

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*	$00\frac{1}{4}\ P_c$
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*	$0\frac{1}{2}0\ I2z$
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 $P4_22_12$

2	*a*	2.22		*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*	$0\frac{1}{2}0\ (..2\ CI1z)_c$
4	*e*	..2		$P4_2/mnm\ f$	.*n*. *I*2*xx*
4	*f*				$00\frac{1}{2}\ .n.\ I2xx$
8	*g*	1	*	$P4_22_12\ g$	$.2_1.\ I2xx2yz$

95 $P4_322$

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 $P4_32_12$

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		*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*	2.22		*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*	2..		*P*4/*mmm g*	$0\frac{1}{2}0\ C_c2z$
8	*g*	..2		*I*4/*mmm h*	*I*4*xx*
8	*h*	.2.		*I*4/*mmm i*	*I*4*x*
8	*i*				$00\frac{1}{2}\ I4x$
8	*j*	..2		*I*4/*mcm h*	$0\frac{1}{2}\frac{1}{4}\ .b.\ C_c2xx$
16	*k*	1	*	*I*422 *k*	*I*4*x*2*yz*

98 $I4_122$

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*				$.2.\ {}^vD2x\bar{x}$

Table 3.4.3.3 (continued)

8	f	.2.	*	$I4_122\ f$	$..22\ {}^{v}TC_{cc}1x$
16	g	1	*	$I4_122\ g$	$.2.\ {}^{v}D2xx2yz$

99 *P4mm*

1	a	4mm		P4/mmm a	P[z]
1	b				$\frac{1}{2}\frac{1}{2}0$ P[z]
2	c	2mm.		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 *P4bm*

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 $P4_2cm$

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 $P4_2nm$

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 *P4cc*

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 *P4nc*

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 $P4_2mc$

2	a	2mm.		P4/mmm a	$P_c[z]$
2	b				$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
2	c	2mm.		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 $P4_2bc$

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		$P4_2/mbc\ h$	$.b2\ C_c2xy[z]$

107 *I4mm*

2	a	4mm		I4/mmm a	I[z]
4	b	2mm.		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 *I4cm*

4	a	4..		P4/mmm a	$C_c[z]$
4	b	2.mm		P4/mmm a	$\frac{1}{2}00\ C_c[z]$
8	c	..m		I4/mcm h	$\frac{1}{2}00\ .b.\ C_c2xx[z]$
16	d	1		I4/mcm k	$..m\ C_c4xy[z]$

109 $I4_1md$

4	a	2mm.		$I4_1/amd\ a$	${}^{v}D[z]$
8	b	.m.	*	$I4_1md\ b$	$..d\ {}^{v}D2x[z]$
16	c	1	*	$I4_1md\ c$	$..d\ {}^{v}D2x2y[z]$

110 $I4_1cd$

8	a	2..		I4/mmm a	$F_c[z]$
16	b	1	*	$I4_1cd\ b$	$.bd\ F_c2xy[z]$

111 $P\bar{4}2m$

1	a	$\bar{4}2m$		P4/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.		P4/mmm a	$\frac{1}{2}00$ C
2	f				$\frac{1}{2}0\frac{1}{2}$ C
2	g	2.mm		P4/mmm g	P2z
2	h				$\frac{1}{2}\frac{1}{2}0$ P2z
4	i	.2.		P4/mmm l	P4x
4	j				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ P4x
4	k				$00\frac{1}{2}$ P4x
4	l				$\frac{1}{2}\frac{1}{2}0$ P4x
4	m	2..		P4/mmm g	$0\frac{1}{2}0$ C2z
4	n	..m	*	$P\bar{4}2m\ n$	P4xxz
8	o	1	*	$P\bar{4}2m\ o$	P4xxz2y

112 $P\bar{4}2c$

2	a	222.		P4/mmm a	$00\frac{1}{4}\ P_c$
2	c				$\frac{1}{2}\frac{1}{2}\frac{1}{4}\ P_c$
2	b	222.		I4/mmm a	$\frac{1}{2}0\frac{1}{4}$ I
2	d				$0\frac{1}{2}\frac{1}{4}$ I
2	e	$\bar{4}..$		P4/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..		P4/mmm g	P_c2z
4	l				$\frac{1}{2}\frac{1}{2}0\ P_c2z$
4	m	2..		I4/mmm e	$0\frac{1}{2}\frac{1}{4}$ I2z
8	n	1	*	$P\bar{4}2c\ n$	$.2.\ P_c4xyz$

Table 3.4.3.3 (continued)

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*
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*	${}^vD$
4	*b*				$00\frac{1}{2}$ ${}^vD$
8	*c*	2..		$I4_1/amd$ *e*	${}^vD2z$
8	*d*	.2.	*	$I\bar{4}2d$ *d*	$\bar{4}$.. ${}^vTF_c1x$
16	*e*	1	*	$I\bar{4}2d$ *e*	.2. ${}^vD4xyz$

Table 3.4.3.3 (continued)

123 $P4/mmm$

1	*a*	$4/mmm$	*	$P4/mmm$ *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*	$mmm.$		$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{2}$ C
2	*f*				$0\frac{1}{2}0$ C
2	*g*	$4mm$	*	$P4/mmm$ *g*	$P2z$
2	*h*				$\frac{1}{2}\frac{1}{2}0$ $P2z$
4	*i*	$2mm.$		$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
4	*j*	$m.2m$	*	$P4/mmm$ *j*	$P4xx$
4	*k*				$00\frac{1}{2}$ $P4xx$
4	*l*	$m2m.$	*	$P4/mmm$ *l*	$P4x$
4	*m*				$00\frac{1}{2}$ $P4x$
4	*n*				$\frac{1}{2}\frac{1}{2}0$ $P4x$
4	*o*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $P4x$
8	*p*	$m..$	*	$P4/mmm$ *p*	$P4x2y$
8	*q*				$00\frac{1}{2}$ $P4x2y$
8	*r*	$..m$	*	$P4/mmm$ *r*	$P4xx2z$
8	*s*	$.m.$	*	$P4/mmm$ *s*	$P4x2z$
8	*t*				$\frac{1}{2}\frac{1}{2}0$ $P4x2z$
16	*u*	1	*	$P4/mmm$ *u*	$P4x2y2z$

124 $P4/mcc$

2	*a*	422		$P4/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*c*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	$4/m..$		$P4/mmm$ *a*	P_c
2	*d*				$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	$2/m..$		$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*f*	222.		$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*g*	4..		$P4/mmm$ *g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
8	*i*	2..		$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*j*	..2		$P4/mmm$ *j*	$00\frac{1}{4}$ P_c4xx
8	*k*	.2.		$P4/mmm$ *l*	$00\frac{1}{4}$ P_c4x
8	*l*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*m*	$m..$	*	$P4/mcc$ *m*	$.c.$ P_c4xy
16	*n*	1	*	$P4/mcc$ *n*	$.c.$ P_c4xy2z

125 $P4/nbm$

2	*a*	422		$P4/mmm$ *a*	C
2	*b*				$00\frac{1}{2}$ C
2	*c*	$\bar{4}2m$		$P4/mmm$ *a*	$0\frac{1}{2}0$ C
2	*d*				$0\frac{1}{2}\frac{1}{2}$ C
4	*e*	$..2/m$		$P4/mmm$ *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..		$P4/mmm$ *g*	$C2z$
4	*h*	$2.mm$		$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
8	*i*	..2		$P4/mmm$ *l*	$C4xx$
8	*j*				$00\frac{1}{2}$ $C4xx$
8	*k*	.2.		$P4/mmm$ *j*	$C4x$
8	*l*				$00\frac{1}{2}$ $C4x$
8	*m*	$..m$	*	$P4/nbm$ *m*	$0\frac{1}{2}0$ $..2$ $C4xxz$
16	*n*	1	*	$P4/nbm$ *n*	$..m$ $C4x2yz$

126 $P4/nnc$

2	*a*	422		$I4/mmm$ *a*	I
2	*b*				$00\frac{1}{2}$ I
4	*c*	222.		$P4/mmm$ *a*	$\frac{1}{2}00$ C_c
4	*d*	$\bar{4}..$		$P4/mmm$ *a*	$\frac{1}{2}0\frac{1}{4}$ C_c
4	*e*	4..		$I4/mmm$ *e*	$I2z$
8	*f*	$\bar{1}$		$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..		$P4/mmm$ *g*	$\frac{1}{2}00$ C_c2z
8	*h*	..2		$I4/mmm$ *h*	$I4xx$
8	*i*	.2.		$I4/mmm$ *i*	$I4x$
8	*j*				$00\frac{1}{2}$ $I4x$
16	*k*	1	*	$P4/nnc$ *k*	$..c$ $I4x2yz$

127 $P4/mbm$

2	*a*	$4/m..$		$P4/mmm$ *a*	C
2	*b*				$00\frac{1}{2}$ C
2	*c*	$m.mm$		$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{2}$ C
2	*d*				$0\frac{1}{2}0$ C
4	*e*	4..		$P4/mmm$ *g*	$C2z$
4	*f*	$2.mm$		$P4/mmm$ *g*	$0\frac{1}{2}0$ $C2z$
4	*g*	$m.2m$	*	$P4/mbm$ *g*	$0\frac{1}{2}0$ $.b.$ $C2xx$
4	*h*				$0\frac{1}{2}\frac{1}{2}$ $.b.$ $C2xx$
8	*i*	$m..$	*	$P4/mbm$ *i*	$..m$ $C4xy$
8	*j*				$00\frac{1}{2}$ $..m$ $C4xy$
8	*k*	$..m$	*	$P4/mbm$ *k*	$0\frac{1}{2}0$ $.b.$ $C2xx2z$
16	*l*	1	*	$P4/mbm$ *l*	$..m$ $C4xy2z$

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

Table 3.4.3.3 (continued)

4	*c*	4..		*P*4/*nmm c*	$0\frac{1}{2}0$ (..2 *CI*1*z*)$_c$
8	*d*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	2..		*P*4/*mmm g*	C_c2z
8	*f*	..2		*I*4/*mcm h*	$00\frac{1}{4}$.*b*. C_c2xx
16	*g*	1	*	*P*4/*ncc g*	..*c*2 C_c4xyz

131 $P4_2/mmc$

2	*a*	*mmm*.		*P*4/*mmm a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	*mmm*.		*I*4/*mmm a*	$0\frac{1}{2}0$ *I*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	$\bar{4}m2$		*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*mm*.		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2*mm*.		*I*4/*mmm e*	$0\frac{1}{2}0$ *I*2*z*
4	*j*	*m*2*m*.	*	$P4_2/mmc$ *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		*P*4/*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*		*P*4/*mmm a*	P_c
2	*c*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*b*	$\bar{4}2m$		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*e*	222.		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*f*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*g*	2.*mm*		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	*m*.2*m*	*	$P4_2/mcm$ *i*	.2. P_c2xx
4	*j*				$00\frac{1}{2}$ .2. P_c2xx
8	*k*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*l*	.2.		*P*4/*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.		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*b*	222.		*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*c*	2.22		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	C_c
8	*e*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*g*	2..		*P*4/*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		*I*4/*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*	$\bar{4}2m$		*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*	2.22		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	..2/*m*		*I*4/*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*		*I*4/*mmm e*	*I*2*z*
8	*h*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*i*	.2.		*I*4/*mmm i*	*I*4*x*
8	*j*				$00\frac{1}{2}$ *I*4*x*
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 *I*4*xxz*
16	*n*	1	*	$P4_2/nnm$ *n*	..2 *I*4*xxz*2*y*

135 $P4_2/mbc$

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

136 $P4_2/mnm$

2	*a*	*m*.*mm*		*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*	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 *CI*1*z*)$_c$
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*

Table 3.4.3.3 (continued)

138 $P4_2/ncm$

4	*a*	2.22		$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}$..		$P4/mmm$ *a*	C_c
4	*c*	..2/*m*		$I4/mmm$ *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*		$P4/nmm$ *c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
8	*f*	2..		$P4/mmm$ *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*	$\frac{1}{4}\frac{3}{4}\frac{1}{4}$ $\bar{4}$.. $F2xxz$
16	*j*	1	*	$P4_2/ncm$ *j*	..*m*2 C_c4xyz

139 $I4/mmm$

2	*a*	4/*mmm*	*	$I4/mmm$ *a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	*mmm*.		$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}m2$		$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4*mm*	*	$I4/mmm$ *e*	$I2z$
8	*f*	..2/*m*		$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2*mm*.		$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*.2*m*	*	$I4/mmm$ *h*	$I4xx$
8	*i*	*m*2*m*.	*	$I4/mmm$ *i*	$I4x$
8	*j*				$\frac{1}{2}\frac{1}{2}0$ $I4x$
16	*k*	..2		$P4/mmm$ *l*	$0\frac{1}{2}\frac{1}{4}$ C_c4xx
16	*l*	*m*..	*	$I4/mmm$ *l*	$I4x2y$
16	*m*	..*m*	*	$I4/mmm$ *m*	$I4xx2z$
16	*n*	.*m*.	*	$I4/mmm$ *n*	$I4x2z$
32	*o*	1	*	$I4/mmm$ *o*	$I4x2y2z$

140 $I4/mcm$

4	*a*	422		$P4/mmm$ *a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}2m$		$P4/mmm$ *a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*c*	4/*m*..		$P4/mmm$ *a*	C_c
4	*d*	*m*.*mm*		$P4/mmm$ *a*	$0\frac{1}{2}0$ C_c
8	*e*	..2/*m*		$P4/mmm$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	4..		$P4/mmm$ *g*	C_c2z
8	*g*	2.*mm*		$P4/mmm$ *g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*.2*m*	*	$I4/mcm$ *h*	$0\frac{1}{2}0$.*b*. C_c2xx
16	*i*	..2		$P4/mmm$ *l*	$00\frac{1}{4}$ C_c4xx
16	*j*	.2.		$P4/mmm$ *j*	$00\frac{1}{4}$ C_c4x
16	*k*	*m*..	*	$I4/mcm$ *k*	..*m* C_c4xy
16	*l*	..*m*	*	$I4/mcm$ *l*	$0\frac{1}{2}\frac{1}{4}$.*b*. C_c4xxz
32	*m*	1	*	$I4/mcm$ *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*	$\bar{4}$..		$I4/mmm$ *a*	F_c
8	*b*	2.22		$I4/mmm$ *a*	$00\frac{1}{4}$ F_c
16	*c*	$\bar{1}$		$I4/mmm$ *a*	$0\frac{1}{4}\frac{1}{8}$ I_2
16	*d*	2..		$I4/mmm$ *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 $P3$

1	*a*	3..		$P6/mmm$ *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*	1		$P\bar{6}$ *j*	$P3xy[z]$

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 $R3$ (Hexagonal axes)

3	*a*	3.		$R\bar{3}m$ *a*	$R[z]$
9	*b*	1	*	$R3$ *b*	$R3xy[z]$

146 $R3$ (Rhombohedral axes)

1	*a*	3.		$R\bar{3}m$ *a*	$P[xxx]$
3	*b*	1	*	$R3$ *b*	$P3yz[xxx]$

147 $P\bar{3}$

1	*a*	$\bar{3}$..		$P6/mmm$ *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*	$\bar{1}$		$P6/mmm$ *f*	*N*
3	*f*				$00\frac{1}{2}$ *N*
6	*g*	1	*	$P\bar{3}$ *g*	$P6xyz$

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*	$R2z$
9	*d*	$\bar{1}$		$R\bar{3}m$ *e*	$00\frac{1}{2}$ *M*
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*	$P6xyz$

Table 3.4.3.3 (continued)

149 *P*312

1	*a*	3.2		*P*6/*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..		*P*6/*mmm e*	*P*2*z*
2	*h*				$\frac{1}{3}\frac{2}{3}0$ *P*2*z*
2	*i*				$\frac{2}{3}\frac{1}{3}0$ *P*2*z*
3	*j*	..2		$P\bar{6}m2$ *j*	$P3x\bar{x}$
3	*k*				$00\frac{1}{2}$ $P3x\bar{x}$
6	*l*	1	*	*P*312 *l*	$P3x\bar{x}2yz$

150 *P*321

1	*a*	32.		*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*	.2.		$P\bar{6}2m$ *f*	*P*3*x*
3	*f*				$00\frac{1}{2}$ *P*3*x*
6	*g*	1	*	*P*321 *g*	*P*3*x*2*yz*

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*	*R*2*z*
9	*d*	.2	*	*R*32 *d*	*R*3*x*
9	*e*				$00\frac{1}{2}$ *R*3*x*
18	*f*	1	*	*R*32 *f*	*R*3*x*2*yz*

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*	*P*2*xxx*
3	*d*	.2	*	*R*32 *d*	$P3x\bar{x}$
3	*e*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ $P3x\bar{x}$
6	*f*	1	*	*R*32 *f*	$P3x\bar{x}2yz$

156 *P*3*m*1

1	*a*	3*m*.		*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*	.*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*		*P*6/*mmm a*	*P*[*z*]
2	*b*	3..		*P*6/*mmm c*	*G*[*z*]
3	*c*	..*m*		$P\bar{6}2m$ *f*	*P*3*x*[*z*]
6	*d*	1		$P\bar{6}2m$ *j*	*P*3*x*2*y*[*z*]

158 *P*3*c*1

2	*a*	3..		*P*6/*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..		*P*6/*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*	*	*R*3*m b*	$R3x\bar{x}[z]$
18	*c*	1	*	*R*3*m 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*	*	*R*3*m b*	*P*3*z*[*xxx*]
6	*c*	1	*	*R*3*m c*	*P*3*z*2*y*[*xxx*]

161 *R*3*c* (Hexagonal axes)

6	*a*	3.		$R\bar{3}m$ *a*	$'R_c[z]$
18	*b*	1	*	*R*3*c b*	.*c* $'R_c3xy[z]$

161 *R*3*c* (Rhombohedral axes)

2	*a*	3.		$R\bar{3}m$ *a*	*I*[*xxx*]
6	*b*	1	*	*R*3*c b*	.*n* *I*3*yz*[*xxx*]

162 $P\bar{3}1m$

1	*a*	$\bar{3}$.*m*		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
2	*c*	3.2		*P*6/*mmm c*	*G*
2	*d*				$00\frac{1}{2}$ *G*
2	*e*	3.*m*		*P*6/*mmm e*	*P*2*z*
3	*f*	..2/*m*		*P*6/*mmm f*	*N*

Table 3.4.3.3 (continued)

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 $P\bar{3}1c$

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 $P\bar{3}m1$

1	*a*	$\bar{3}m$.		$P6/mmm$ *a*	P
1	*b*				$00\frac{1}{2}$ P
2	*c*	3*m*.		$P6/mmm$ *e*	$P2z$
2	*d*	3*m*.	*	$P\bar{3}m1$ *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 $P\bar{3}c1$

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

3	*a*	$\bar{3}m$	*	$R\bar{3}m$ *a*	R
3	*b*				$00\frac{1}{2}$ R
6	*c*	3*m*	*	$R\bar{3}m$ *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 $R\bar{3}m$ (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*	3*m*	*	$R\bar{3}m$ *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 $R\bar{3}c$ (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 $R\bar{3}c$ (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 $P6$

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 $P6_1$

6	*a*	1	*	$P6_1$ *a*	3_12_1.. $P_{Cc}E_C{}^+Q_c1xy[z]$

170 $P6_5$

6	*a*	1	*	$P6_1a$	3_22_1.. $P_{Cc}E_C{}^-Q_c1xy[z]$

171 $P6_2$

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 $P6_4$

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 $P6_3$

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 $P\bar{6}$

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

Table 3.4.3.3 (continued)

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

175 *P*6/*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 *P*622

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 *P*6*mm*

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]

Table 3.4.3.3 (continued)

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*	3*m*.		$P6/mmm$ *a*	$P_c[z]$
2	*b*	3*m*.		$P6_3/mmc$ *c*	$E[z]$
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*	3*m*.		$P6/mmm$ *e*	$P2z$
2	*h*				$\frac{1}{3}\frac{2}{3}0\ P2z$
2	*i*				$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	*mm*2	*	$P\bar{6}m2$ *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*	*m*2*m*	*	$P\bar{6}2m$ *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*	6*mm*	*	$P6/mmm$ *e*	$P2z$
3	*f*	*mmm*	*	$P6/mmm$ *f*	N
3	*g*				$00\frac{1}{2}\ N$
4	*h*	3*m*.	*	$P6/mmm$ *h*	$G2z$
6	*i*	2*mm*	*	$P6/mmm$ *i*	$N2z$
6	*j*	*m*2*m*	*	$P6/mmm$ *j*	$P6x$
6	*k*				$00\frac{1}{2}\ P6x$
6	*l*	*mm*2	*	$P6/mmm$ *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*	$.c.\ P_c6xy2z$

Table 3.4.3.3 (continued)

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*	*m*2*m*	*	$P6_3/mcm\ g$	$00\frac{1}{4}$ ..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*	3*m*.		$P6/mmm\ e$	P_c2z
4	*f*	3*m*.	*	$P6_3/mmc\ f$	$E2z$
6	*g*	.2/*m*.		$P6/mmm\ f$	N_c
6	*h*	*mm*2	*	$P6_3/mmc\ h$	$00\frac{1}{4}$ .2. $P_c3x\bar{x}$
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.		$P\bar{4}3m\ e$	$P4xxx$
6	*f*	2..		$Pm\bar{3}m\ e$	$P6z$
6	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
6	*g*	2..		$Pm\bar{3}\ f$	.3. $J2x$
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. $J2x$
12	*j*	1	*	$P23\ j$	$P6z2xy$

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.		$F\bar{4}3m\ e$	$F4xxx$
24	*f*	2..		$Fm\bar{3}m\ e$	$F6z$
24	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F6z$
48	*h*	1	*	$F23\ h$	$F6z2xy$

197 *I*23

2	*a*	23.		$Im\bar{3}m\ a$	I
6	*b*	222..		$Im\bar{3}m\ b$	J^*
8	*c*	.3.		$I\bar{4}3m\ c$	$I4xxx$
12	*d*	2..		$Im\bar{3}m\ e$	$I6z$
12	*e*	2..		$Im\bar{3}\ e$	.3. J^*2x
24	*f*	1	*	$I23\ f$	$I6z2xy$

198 $P2_13$

4	*a*	.3.	*	$P2_13\ a$	$2_12_1..\ FY1xxx$
12	*b*	1	*	$P2_13\ b$	$2_12_1..\ FY1xxx3yz$

199 $I2_13$

8	*a*	.3.	*	$I2_13\ a$	$2_12_1..\ P_2Y^*1xxx$
12	*b*	2..	*	$I2_13\ b$	$2_13.\ SV1z$
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..		$Pm\bar{3}m\ e$	$P6z$
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
6	*f*	*mm*2..	*	$Pm\bar{3}\ f$	.3. $J2x$
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. $J2x$
8	*i*	.3.		$Pm\bar{3}m\ g$	$P8xxx$
12	*j*	*m*..	*	$Pm\bar{3}\ j$	$P6z2x$
12	*k*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z2x$
24	*l*	1	*	$Pm\bar{3}\ l$	$P6z2x2y$

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 $I4xxx$
12	*f*	2..		$Im\bar{3}m\ e$	$I6z$
12	*g*	2..		$Im\bar{3}\ e$	.3. J^*2x
24	*h*	1	*	$Pn\bar{3}\ h$	*n*.. $I6z2xy$

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..		$Fm\bar{3}m\ e$	$F6z$
32	*f*	.3.		$Fm\bar{3}m\ f$	$F8xxx$
48	*g*	2..		$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
48	*h*	*m*..	*	$Fm\bar{3}\ h$	$F6z2x$
96	*i*	1	*	$Fm\bar{3}\ i$	$F6z2x2y$

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 $D4xxx$

Table 3.4.3.3 (continued)

48	f	2..		$Fd\bar{3}m$ f	D6z
96	g	1	*	$Fd\bar{3}$ g	d.. D6z2xy

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	mm2..		$Im\bar{3}m$ e	I6z
12	e	mm2..	*	$Im\bar{3}$ e	.3. J*2x
16	f	.3.		$Im\bar{3}m$ f	I8xxx
24	g	m..	*	$Im\bar{3}$ g	I6z2x
48	h	1	*	$Im\bar{3}$ h	I6z2x2y

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.. F2xxx
24	d	1	*	$Pa\bar{3}$ d	bc.. F6xyz

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_2$2xxx
24	d	2..	*	$Ia\bar{3}$ d	$.\bar{3}.$ $J_2S^*V^*1x$
48	e	1	*	$Ia\bar{3}$ e	22.. $P_2$6xyz

207 P432

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
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_2$6z
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

Table 3.4.3.3 (continued)

24	*f*	2..	*	$I4_132\ f$	.3. *V*2*z*
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*	*	$P\bar{4}3m\ e$	*P*4*xxx*
6	*f*	2.*mm*		$Pm\bar{3}m\ e$	*P*6*z*
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
12	*h*	2..		$Pm\bar{3}m\ h$	.3. *J*4*x*
12	*i*	..*m*	*	$P\bar{4}3m\ i$	*P*6*z*2*xx*
24	*j*	1	*	$P\bar{4}3m\ j$	*P*6*z*2*xx*2*y*
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*	*	$F\bar{4}3m\ e$	*F*4*xxx*
24	*f*	2.*mm*		$Fm\bar{3}m\ e$	*F*6*z*
24	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F6z$
48	*h*	..*m*	*	$F\bar{4}3m\ h$	*F*6*z*2*xx*
96	*i*	1	*	$F\bar{4}3m\ i$	*F*6*z*2*xx*2*y*
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*	*	$I\bar{4}3m\ c$	*I*4*xxx*
12	*d*	$\bar{4}..$		$Im\bar{3}m\ d$	W^*
12	*e*	2.*mm*		$Im\bar{3}m\ e$	*I*6*z*
24	*f*	2..		$Im\bar{3}m\ g$	.3. J^*4x
24	*g*	..*m*	*	$I\bar{4}3m\ g$	*I*6*z*2*xx*
48	*h*	1	*	$I\bar{4}3m\ h$	*I*6*z*2*xx*2*y*
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_24xxx
48	*f*	2..		$Pm\bar{3}m\ e$	P_26z
48	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
96	*h*	1	*	$F\bar{4}3c\ h$	..*n* P_26z2xy
220 $I\bar{4}3d$					
12	*a*	$\bar{4}..$	*	$I\bar{4}3d\ a$	*S*
12	*b*				$'S$
16	*c*	.3.	*	$I\bar{4}3d\ c$	$\bar{4}..\ I_2Y^{**}1xxx$
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*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z$
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*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P12xx$
24	*k*	*m*..	*	$Pm\bar{3}m\ k$	*P*6*z*4*x*
24	*l*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6z4x$
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^*4x
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*

Table 3.4.3.3 (continued)

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*	$.3m$	*	$Pn\bar{3}m\ e$	$..2\ I4xxx$
12	*f*	2.22		$Im\bar{3}m\ d$	W^*
12	*g*	$2.mm$		$Im\bar{3}m\ e$	$I6z$
24	*h*	$2..$		$Im\bar{3}m\ g$	$.3.\ J^*4x$
24	*i*	$..2$	*	$Pn\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ \bar{4}..\ F6x\bar{x}$
24	*j*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}\ \bar{4}..\ F6x\bar{x}$
24	*k*	$..m$	*	$Pn\bar{3}m\ k$	$..2\ I6z2xx$
48	*l*	1	*	$Pn\bar{3}m\ l$	$..2\ I6z2xx2y$

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*	$4m.m$	*	$Fm\bar{3}m\ e$	$F6z$
32	*f*	$.3m$	*	$Fm\bar{3}m\ f$	$F8xxx$
48	*g*	$2.mm$		$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
48	*h*	$m.m2$	*	$Fm\bar{3}m\ h$	$F12xx$
48	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ F12xx$
96	*j*	$m..$	*	$Fm\bar{3}m\ j$	$F6z4x$
96	*k*	$..m$	*	$Fm\bar{3}m\ k$	$F6z4xx$
192	*l*	1	*	$Fm\bar{3}m\ l$	$F6z4x2y$

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*	$mm2..$		$Pm\bar{3}m\ e$	P_26z
48	*f*	$4..$		$Pm\bar{3}m\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_26z$
64	*g*	$.3.$		$Pm\bar{3}m\ g$	P_28xxx
96	*h*	$..2$		$Pm\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_212xx$
96	*i*	$m..$	*	$Fm\bar{3}c\ i$	$..2\ P_26z2x$
192	*j*	1	*	$Fm\bar{3}c\ j$	$..2\ P_26z2x2y$

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*	$.3m$	*	$Fd\bar{3}m\ e$	$..2\ D4xxx$
48	*f*	$2.mm$	*	$Fd\bar{3}m\ f$	$D6z$
96	*g*	$..m$	*	$Fd\bar{3}m\ g$	$..2\ D6z2xx$
96	*h*	$..2$	*	$Fd\bar{3}m\ h$	$\bar{4}..\ T6x\bar{x}$
192	*i*	1	*	$Fd\bar{3}m\ i$	$..2\ D6z2xx2y$

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_26z
96	*g*	$..2$	*	$Fd\bar{3}c\ g$	$\frac{1}{8}\frac{1}{8}\frac{1}{8}\ \bar{4}2..\ F_23x\bar{x}$
192	*h*	1	*	$Fd\bar{3}c\ h$	$d.2\ I_26z2xy$

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*	$4m.m$	*	$Im\bar{3}m\ e$	$I6z$
16	*f*	$.3m$	*	$Im\bar{3}m\ f$	$I8xxx$
24	*g*	$mm2..$	*	$Im\bar{3}m\ g$	$.3.\ J^*4x$
24	*h*	$m.m2$	*	$Im\bar{3}m\ h$	$I12xx$
48	*i*	$..2$	*	$Im\bar{3}m\ i$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ 4..\ P_26x\bar{x}$
48	*j*	$m..$	*	$Im\bar{3}m\ j$	$I6z4x$
48	*k*	$..m$	*	$Im\bar{3}m\ k$	$I6z4xx$
96	*l*	1	*	$Im\bar{3}m\ l$	$I6z4x2y$

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	*	$Ia\bar{3}d\ h$	$\bar{4}a..\ I_26xyz$

crystal structures (Smirnova, 1962), of Patterson diagrams (Koch & Hellner, 1971), of Dirichlet domains (Koch, 1973, 1984) and of sphere packings for subperiodic groups (Koch & Fischer, 1978*b*).

The 30 lattice complexes in two-dimensional space correspond uniquely to the 'henomeric types of dot pattern' introduced by Grünbaum and Shephard (*cf. e.g.* Grünbaum & Shephard, 1981; Grünbaum, 1983).

3.4.4.2. Relations between crystal structures

Different crystal structures frequently show the same geometrical arrangement for some of their atoms, even though their space groups do not belong to the same type. In such cases, the corresponding Wyckoff positions either belong to the same lattice complex or there exists a close relationship between them, *e.g.* a limiting-complex relation.

Examples

(1) The Fe atoms in pyrite FeS_2 occupy Wyckoff position $4a$ $.\bar{3}.$ 0, 0, 0 of $Pa\bar{3}$ (descriptive symbol F) that belongs to the invariant lattice complex $Fm\bar{3}m$ a. Accordingly, the Fe atoms in pyrite form a face-centred cubic lattice, as do the Cu atoms in the element structure of copper.

(2) Cuprite Cu_2O crystallizes with symmetry $Pn\bar{3}m$. The oxygen atoms occupy Wyckoff position $2a$ $\bar{4}3m$ 0, 0, 0 (descriptive symbol I) and the copper atoms position $4b$ $.\bar{3}m$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ F). Position $2a$ belongs to lattice complex $Im\bar{3}m$ a and position $4b$ to $Fm\bar{3}m$ a. Therefore, the O atoms form a body-centred cubic lattice like the W atoms in the structure of tungsten, and the copper atoms form a face-centred cubic lattice. The tungsten configuration is shifted by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ with respect to the copper configuration.

(3) K_2NaAlF_6 (elpasolite, *cf.* Morss, 1974) and $K_2PbNi(NO_2)_6$ (*cf.* Takagi *et al.*, 1975) crystallize with symmetry $Fm\bar{3}m$ and $Fm\bar{3}$, respectively.

K_2NaAlF_6

Al	$4a$	$m\bar{3}m$	0, 0, 0	F
Na	$4b$	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	$8c$	$\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
F	$24e$	$4m.m$	x, 0, 0	$F6z$
			$x = 0.219$	

$K_2PbNi(NO_2)_6$

Ni	$4a$	$m\bar{3}.$	0, 0, 0	F
Pb	$4b$	$m\bar{3}.$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	$8c$	23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
N	$24e$	$mm2..$	x, 0, 0	$F6z$
			$x = 0.1966$	
O	$48h$	$m..$	0, y, z	$F6z2x$

As the descriptive lattice-complex symbols for the various atomic positions show immediately, the two crystal structures are very similar. The only difference originates from the replacement of the fluorine atoms in elpasolite by NO_2 groups in $K_2PbNi(NO_2)_6$, which causes the symmetry reduction from $Fm\bar{3}m$ to $Fm\bar{3}$.

(4) The crystal structure of CoU (Baenziger *et al.*, 1950) may be interpreted as a slightly distorted CsCl (or β-brass, CuZn)-type structure. CsCl corresponds to Wyckoff positions $1a$ and $1b$ of $Pm\bar{3}m$ with descriptive symbols P and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ P, respectively; Co and U both occupy Wyckoff position $8a$ $.3.$ x, x, x of $I2_13$ with $x = 0.0347$ for U and $x = 0.294$ for Co. As the descriptive symbol $2_12_1..$ P_2Y^*1xxx shows, this Wyckoff position belongs to a Weissenberg complex with two invariant limiting complexes, namely P ($Pm\bar{3}m$ a) and Y^* ($I4_132$ a). $x = 0$ corresponds to P_2, $x = \frac{1}{4}$ to $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2, $x = \frac{1}{8}$ to ${}^+Y^*$ and $x = \frac{7}{8}$ to ${}^-Y^*$. Consequently, the uranium and cobalt atoms form approximately a P_2 and a $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2 configuration, respectively.

Publications by Hellner (1965, 1976*a*,*b*,*c*, 1977, 1979), Loeb (1970), Smirnova & Vasserman (1971), Sakamoto & Takahasi (1971), Niggli (1971), Fischer & Koch (1974*b*), Hellner *et al.* (1981) and Hellner & Sowa (1985) refer to this aspect.

3.4.4.3. Reflection conditions

Wyckoff positions belonging to the same lattice complex show analogous reflection conditions. Therefore, lattice complexes have also been used to check the reflection conditions for all Wyckoff positions in the space-group tables of this volume.

Example

The lattice complex oF consists of all face-centred point lattices with orthorhombic symmetry. For its characteristic Wyckoff position $Fmmm$ $4a$, only the general conditions for reflections hkl in space group $Fmmm$ are valid, namely $h + k$, $h + l$, $k + l = 2n$ (*cf.* Chapter 2.3). The non-characteristic Wyckoff position $Ccce$ $4a$ also belongs to this lattice complex. The general reflection condition for $Ccce$ is hkl: $h + k = 2n$. This has to be combined with $k + l = 2n$, the special condition for Wyckoff position a. Together the two conditions produce $h + l = 2n$, the third condition for a face-centred point lattice.

The descriptive symbols may supply information on the reflection conditions. If the symbol does not contain any distribution-symmetry part, the reflection conditions of the Wyckoff position are indicated by the symbol of the invariant lattice complex in the central part (*e.g.* $P4/nmm$ g: $C4xx$ shows that the reflection condition is that of a C lattice, hkl: $h + k = 2n$). In cases where the site set consists of only one point, *i.e.* the Wyckoff position belongs to a Weissenberg complex, all conditions for general reflections hkl that may arise from special choices of the coordinates can be read from the central part of the symbol (*e.g.* $P4/nmm$ c: $0\frac{1}{2}0$ $..2$ $CI1z$ indicates that, by special choice of z, either hkl: $h + k = 2n$ or hkl: $h + k + l = 2n$ may be produced).

3.4.4.4. Phase transitions

If a crystal undergoes a phase transition from a high- to a low-symmetry modification, the transition may be connected with a group–subgroup transition. In such cases, the comparison of the lattice complexes corresponding to the Wyckoff positions of the original space group on the one hand and of its various subgroups on the other hand very often shows which of these subgroups are suitable for the low-symmetry modification.

This kind of procedure will be demonstrated with the aid of the space group $R\bar{3}m$ and its three *translationengleiche* subgroups with index 2, namely $R32$, $R\bar{3}$ and $R3m$. In the course of the restriction to a subgroup, the Wyckoff positions of $R\bar{3}m$ behave differently:

The descriptive symbols R and $00\frac{1}{2}R$ refer to Wyckoff positions $R\bar{3}m$ 3a and 3b as well as to Wyckoff positions $R32$ 3a and 3b and $R\bar{3}$ 3a and 3b. Therefore, all corresponding point configurations and atomic arrangements remain unchanged in these subgroups. In subgroup $R3m$, however, the respective Wyckoff position is 3a with descriptive symbol $R[z]$, *i.e.* a shift parallel to [001] of the entire point configuration is allowed.

The descriptive symbol $R2z$ for $R\bar{3}m$ 6c also occurs for $R32$ 6c and $R\bar{3}$ 6c. Again, neither subgroup allows any deformations of the corresponding point configurations or atomic arrangements. Symmetry reduction to $R3m$, however, yields a splitting of each $R2z$ configuration into two $R[z]$ configurations. The two z parameters may be chosen independently.

As M and $00\frac{1}{2}M$ are the descriptive symbols not only of $R\bar{3}m$ 9e and 9d but also of $R\bar{3}$ 9e and 9d, $R\bar{3}$ does not enable any deformation of the corresponding atomic arrangements. In $R32$ and in $R3m$, however, the respective point configurations may be differently deformed, as the descriptive symbols show: $R3x$ and $00\frac{1}{2}R3x$ ($R32$ 9d and 9e), $R3x\bar{x}[z]$ ($R3m$ 9b).

Wyckoff positions $R\bar{3}m$ 18f and 18g ($R6x$ and $00\frac{1}{2}R6x$) correspond to $R32$ 9d and 9e ($R3x$ and $00\frac{1}{2}R3x$), to $R\bar{3}$ 18f ($R6xyz$), and to $R3m$ 18c ($R3x\bar{x}2y[z]$). In $R32$, the hexagons 6x around the points of the R lattice are split into two oppositely oriented triangles 3x, which may have different size. In $R\bar{3}$ and in $R3m$, the hexagons may be differently deformed.

Wyckoff position $R\bar{3}m$ 18h ($R6x\bar{x}z$) corresponds to sets of trigonal antiprisms around the points of an R lattice. These antiprisms may be distorted in $R32$ 18f ($R3x2yz$) or rotated in $R\bar{3}$ 18f ($R6xyz$). In $R3m$ 9b ($R3x\bar{x}[z]$), each antiprism is split into two parallel triangles that may differ in size.

In each of the three subgroups, any point configuration belonging to the general position $R\bar{3}m$ 36i splits into two parts. Each of these parts may be differently deformed.

3.4.4.5. Incorrect space-group assignment

In the literature, some crystal structures are still described within space groups that are only subgroups of the correct symmetry groups. Many such mistakes (but not all of them) could be avoided by simply looking at the lattice complexes (and their descriptive symbols) that correspond to the Wyckoff positions of the different kinds of atoms. Whenever the same (or an analogous) lattice-complex description of a crystal structure is also possible within a supergroup, then the crystal structure has at least that symmetry.

Examples

(1) The crystal structure of β-$LiRhO_2$ has been refined in space group $F4_132$ (*cf.* Hobbie & Hoppe, 1986).

Rh	16c	.32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	T
Li	16d	.32	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}T$
O	32e	.3.	x,x,x	..2 $D4xxx$

The same atomic arrangement is possible in the supergroup $Fd\bar{3}m$ of $F4_132$, as can easily be read from Table 3.4.3.3:

Rh	16c	$.\bar{3}m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	T
Li	16d	$.\bar{3}m$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}T$
O	32e	$.3m$	x,x,x	..2 $D4xxx$

Therefore, β-$LiRhO_2$ should be described in $Fd\bar{3}m$.

(2) $KIAs_4O_6$ (Pertlik, 1988) has been described with symmetry $P622$.

I	1a	622	0, 0, 0	P
K	1b	622	$0,0,\frac{1}{2}$	$00\frac{1}{2}P$
As	4h	3..	$\frac{1}{3},\frac{2}{3},z$	$G2z$
O	6i	2..	$\frac{1}{2},0,z$	$N2z$

Space group $P6/mmm$ allows the same atomic arrangement:

I	1a	$6/mmm$	0, 0, 0	P
K	1b	$6/mmm$	$0,0,\frac{1}{2}$	$00\frac{1}{2}P$
As	4h	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$G2z$
O	6i	$2mm$	$\frac{1}{2},0,z$	$N2z$

Therefore, $KIAs_4O_6$ should be described in $P6/mmm$.

3.4.4.6. Application of descriptive lattice-complex symbols

Descriptive symbols of lattice complexes – at least those of the invariant lattice complexes – have been used for the description of crystal structures (*cf.* Section 3.4.4.2 and the literature cited there), for the nomenclature of three-periodic surfaces (von Schnering & Nesper, 1987) and in connection with orbifolds of space groups (Johnson *et al.*, 2001).

3.4.4.7. Weissenberg complexes

In general, each lattice complex involves point configurations that cannot be related to any crystal structure because the shortest distances between the atoms in a corresponding arrangement would become too small. Only the 67 Weissenberg complexes (*cf.* Section 3.4.1.5.2) form an exception from this rule. Assuming that the metrical parameters are chosen adequately, each point configuration stemming from a Weissenberg complex may, in principle, refer to the arrangement of some atoms in a crystal structure. In case of the 36 invariant lattice complexes this property is immediately evident. The further 31 Weissenberg complexes have one or more degrees of freedom (*cf.* Section 3.4.1.5.2 and Table 3.4.1.1). Nevertheless, varying the corresponding free coordinate parameters never results in point configurations with infinitesimally small distances.

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