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1.4. Symmetry in reciprocal space

By U. Shmueli

with Appendix 1.4.2 by U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve

1.4.1. Introduction

Crystallographic symmetry, as reflected in functions on reciprocal space, can be considered from two complementary points of view.

(1) One can assume the existence of a certain permissible symmetry of the density function of crystalline (scattering) matter, a function which due to its three-dimensional periodicity can be expanded in a triple Fourier series (*e.g.* Bragg, 1966), and inquire about the effects of this symmetry on the Fourier coefficients – the structure factors. Since there exists a one-to-one correspondence between the triplets of summation indices in the Fourier expansion and vectors in the reciprocal lattice (Ewald, 1921), the above approach leads to consequences of the symmetry of the density function which are relevant to the representation of its Fourier image in reciprocal space. The symmetry properties of these Fourier coefficients, which are closely related to the crystallographic experiment, can then be readily established.

This traditional approach, the essentials of which are the basis of Sections 4.5–4.7 of Volume I (*IT* I, 1952), and which was further developed in the works of Buerger (1949, 1960), Waser (1955), Bertaut (1964) and Wells (1965), is one of the cornerstones of crystallographic practice and will be followed in the present chapter, as far as the basic principles are concerned.

(2) The alternative approach, proposed by Bienenstock & Ewald (1962), also presumes a periodic density function in crystal space and its Fourier expansion associated with the reciprocal. However, the argument starts from the Fourier coefficients, taken as a discrete set of complex functions, and linear transformations are sought which leave the magnitudes of these functions unchanged; the variables on which these transformations operate are h, k, l and φ – the Fourier summation indices (*i.e.*, components of a reciprocal-lattice vector) and the phase of the Fourier coefficient, respectively. These transformations, or the groups they constitute, are then interpreted in terms of the symmetry of the density function in direct space. This direct analysis of symmetry in reciprocal space will also be discussed.

We start the next section with a brief discussion of the point-group symmetries of associated direct and reciprocal lattices. The weighted reciprocal lattice is then briefly introduced and the relation between the values of the weight function at symmetry-related points of the weighted reciprocal lattice is discussed in terms of the Fourier expansion of a periodic function in crystal space. The remaining part of Section 1.4.2 is devoted to the formulation of the Fourier series and its coefficients (values of the weight function) in terms of space-group-specific symmetry factors, an extensive tabulation of which is presented in Appendix 1.4.3. This is a revised version of the structure-factor tables given in Sections 4.5–4.7 of Volume I (*IT* I, 1952). Appendix 1.4.4 contains a reciprocal-space representation of the 230 crystallographic space groups and some explanatory material related to these space-group tables is given in Section 1.4.4; the latter are interpreted in terms of the two viewpoints discussed above. The tabular material given in this chapter is compatible with the direct-space symmetry tables given in Volume A (*IT* A, 1983) with regard to the space-group settings and choices of the origin.

Most of the tabular material, the new symmetry-factor tables in Appendix 1.4.3 and the space-group tables in Appendix 1.4.4 have been generated by computer with the aid of a combination of numeric and symbolic programming techniques. The algorithm underlying this procedure is briefly summarized in Appendix 1.4.1. Appendix 1.4.2 deals with computer-adapted space-group symbols, including the set of symbols that were used in the preparation of the present tables.

1.4.2. Effects of symmetry on the Fourier image of the crystal

1.4.2.1. *Point-group symmetry of the reciprocal lattice*

Regarding the reciprocal lattice as a collection of points generated from a given direct lattice, it is fairly easy to see that each of the two associated lattices must have the same point-group symmetry. The set of all the rotations that bring the direct lattice into self-coincidence can be thought of as interchanging equivalent families of lattice planes in all the permissible manners. A family of lattice planes in the direct lattice is characterized by a common normal and a certain interplanar distance, and these two characteristics uniquely define the direction and magnitude, respectively, of a vector in the reciprocal lattice, as well as the lattice line associated with this vector and passing through the origin. It follows that any symmetry operation on the direct lattice must also bring the reciprocal lattice into self-coincidence, *i.e.* it must also be a symmetry operation on the reciprocal lattice. The roles of direct and reciprocal lattices in the above argument can of course be interchanged without affecting the conclusion.

The above elementary considerations recall that for any point group (not necessarily the full point group of a lattice), the operations which leave the lattice unchanged must also leave unchanged its associated reciprocal. This equivalence of point-group symmetries of the associated direct and reciprocal lattices is fundamental to crystallographic symmetry in reciprocal space, in both points of view mentioned in Section 1.4.1.

With regard to the effect of any given point-group operation on each of the two associated lattices, we recall that:

(i) If $\boldsymbol{P}$ is a point-group rotation operator acting on the direct lattice (*e.g.* by rotation through the angle α about a given axis), the effect of this rotation on the associated reciprocal lattice is that of applying the inverse rotation operator, $\boldsymbol{P}^{-1}$ (*i.e.* rotation through $-\alpha$ about a direction parallel to the direct axis); this is readily found from the requirement that the scalar product $\mathbf{h}^T\mathbf{r}_L$, where $\mathbf{h}$ and $\mathbf{r}_L$ are vectors in the reciprocal and direct lattices, respectively, remains invariant under the application of a point-group operation to the crystal.

(ii) If our matrix representation of the rotation operator is such that the point-group operation is applied to the direct-lattice (column) vector by *premultiplying* it with the matrix $\boldsymbol{P}$, the corresponding operation on the reciprocal lattice is applied by *postmultiplying* the (row) vector $\mathbf{h}^T$ with the point-group rotation matrix. We can thus write, *e.g.*, $\mathbf{h}^T\mathbf{r}_L = (\mathbf{h}^T\boldsymbol{P}^{-1})(\boldsymbol{P}\mathbf{r}_L) = [(\boldsymbol{P}^{-1})^T\mathbf{h}]^T(\boldsymbol{P}\mathbf{r}_L)$. Note, however, that the orthogonality relationship: $\boldsymbol{P}^{-1} = \boldsymbol{P}^T$ is not satisfied if $\boldsymbol{P}$ is referred to some oblique crystal systems, higher than the orthorhombic.

Detailed descriptions of the 32 crystallographic point groups are presented in the crystallographic and other literature; their complete tabulation is given in Chapter 10 of Volume A (*IT* A, 1983).

1.4.2.2. *Relationship between structure factors at symmetry-related points of the reciprocal lattice*

Of main interest in the context of the present chapter are symmetry relationships that concern the values of a function defined at the points of the reciprocal lattice. Such functions, of crystallographic interest, are Fourier-transform representations of direct-space functions that have the periodicity of the crystal, the structure factor as a Fourier transform of the electron-density function being a representative example (see *e.g.* Lipson & Taylor, 1958). The value of such a function, attached to a reciprocal-lattice point, is called the weight of this point and the set of all such weighted points is often termed the weighted reciprocal lattice. This section deals with a fundamental relationship between functions (weights) associated with reciprocal-lattice points, which are related by point-group symmetry, the weights here considered being the structure factors of Bragg reflections (*cf.* Chapter 1.2).

The electron density, an example of a three-dimensional periodic function with the periodicity of the crystal, can be represented by the Fourier series

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{h}} F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{r}), \qquad (1.4.2.1)$$

where $\mathbf{h}$ is a reciprocal-lattice vector, V is the volume of the (direct) unit cell, $F(\mathbf{h})$ is the structure factor at the point $\mathbf{h}$ and $\mathbf{r}$ is a position vector of a point in direct space, at which the density is given. The summation in (1.4.2.1) extends over all the reciprocal lattice.

Let $\mathbf{r}' = \boldsymbol{P}\mathbf{r} + \mathbf{t}$ be a space-group operation on the crystal, where $\boldsymbol{P}$ and $\mathbf{t}$ are its rotation and translation parts, respectively, and $\boldsymbol{P}$ must therefore be a point-group operator. We then have, by definition, $\rho(\mathbf{r}) = \rho(\boldsymbol{P}\mathbf{r} + \mathbf{t})$ and the Fourier representation of the electron density, at the equivalent position $\boldsymbol{P}\mathbf{r} + \mathbf{t}$, is given by

$$\begin{aligned}\rho(\boldsymbol{P}\mathbf{r} + \mathbf{t}) &= \frac{1}{V}\sum_{\mathbf{h}} F(\mathbf{h}) \exp[-2\pi i \mathbf{h}^T(\boldsymbol{P}\mathbf{r} + \mathbf{t})]\\ &= \frac{1}{V}\sum_{\mathbf{h}} [F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T\mathbf{t})]\\ &\quad \times \exp[-2\pi i (\boldsymbol{P}^T\mathbf{h})^T\mathbf{r}],\end{aligned} \qquad (1.4.2.2)$$

noting that $\mathbf{h}^T\boldsymbol{P} = (\boldsymbol{P}^T\mathbf{h})^T$. Since $\boldsymbol{P}$ is a point-group operator, the vectors $\boldsymbol{P}^T\mathbf{h}$ in (1.4.2.2) must range over all the reciprocal lattice and a comparison of the functional forms of the equivalent expansions (1.4.2.1) and (1.4.2.2) shows that the coefficients of the exponentials $\exp[-2\pi i(\boldsymbol{P}^T\mathbf{h})^T\mathbf{r}]$ in (1.4.2.2) must be the structure factors at the points $\boldsymbol{P}^T\mathbf{h}$ in the reciprocal lattice. Thus

$$F(\boldsymbol{P}^T\mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T\mathbf{t}), \qquad (1.4.2.3)$$

wherefrom it follows that the magnitudes of the structure factors at $\mathbf{h}$ and $\boldsymbol{P}^T\mathbf{h}$ are the same:

$$|F(\boldsymbol{P}^T\mathbf{h})| = |F(\mathbf{h})|, \qquad (1.4.2.4)$$

and their phases are related by

$$\varphi(\boldsymbol{P}^T\mathbf{h}) = \varphi(\mathbf{h}) - 2\pi\mathbf{h}^T\mathbf{t}. \qquad (1.4.2.5)$$

The relationship (1.4.2.3) between structure factors of symmetry-related reflections was first derived by Waser (1955), starting from a representation of the structure factor as a Fourier transform of the electron-density function.

It follows that an application of a point-group transformation to the (weighted) reciprocal lattice leaves the moduli of the structure factors unchanged. The distribution of diffracted intensities obeys, in fact, the same point-group symmetry as that of the crystal. If, however, anomalous dispersion is negligibly small, and the point group of the crystal is noncentrosymmetric, the apparent symmetry of the diffraction pattern will also contain a false centre of symmetry and, of course, all the additional elements generated by the inclusion of this centre. Under these circumstances, the diffraction pattern from a single crystal may belong to one of the eleven centrosymmetric point groups, known as Laue groups (*IT* I, 1952).

According to equation (1.4.2.5), the phases of the structure factors of symmetry-related reflections differ, in the general case, by a phase shift that depends on the translation part of the space-group operation involved. Only when the space group is symmorphic, *i.e.* it contains no translations other than those of the Bravais lattice, will the distribution of the phases obey the point-group symmetry of the crystal. These phase shifts are considered in detail in Section 1.4.4 where their tabulation is presented and the alternative interpretation (Bienenstock & Ewald, 1962) of symmetry in reciprocal space, mentioned in Section 1.4.1, is given.

Equation (1.4.2.3) can be usefully applied to a classification of all the general systematic absences or – as defined in the space-group tables in the main editions of *IT* (1935, 1952, 1983, 1987, 1992) – general conditions for possible reflections. These systematic absences are associated with special positions in the reciprocal lattice – special with respect to the point-group operations $\boldsymbol{P}$ appearing in the relevant relationships. If, in a given relationship, we have $\boldsymbol{P}^T\mathbf{h} = \mathbf{h}$, equation (1.4.2.3) reduces to

$$F(\mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T\mathbf{t}). \qquad (1.4.2.6)$$

Of course, $F(\mathbf{h})$ may then be nonzero only if $\cos(2\pi\mathbf{h}^T\mathbf{t})$ equals unity, or the scalar product $\mathbf{h}^T\mathbf{t}$ is an integer. This well known result leads to a ready determination of lattice absences, as well as those produced by screw-axis and glide-plane translations, and is routinely employed in crystallographic computing. An exhaustive classification of the general conditions for possible reflections is given in the space-group tables (*IT*, 1952, 1983). It should be noted that since the axes of rotation and planes of reflection in the reciprocal lattice are parallel to the corresponding elements in the direct lattice (Buerger, 1960), the component of $\mathbf{t}$ that depends on the location of the corresponding space-group symmetry element in direct space does not contribute to the scalar product $\mathbf{h}^T\mathbf{t}$ in (1.4.2.6), and it is only the intrinsic part of the translation $\mathbf{t}$ (*IT* A, 1983) that usually matters.

It may, however, be of interest to note that some screw axes in direct space cannot give rise to any systematic absences. For example, the general Wyckoff position No. (10) in the space group $Pa\bar{3}$ (No. 205) (*IT* A, 1983) has the coordinates $\bar{y}, \frac{1}{2}+z, \frac{1}{2}-x$, and corresponds to the space-group operation

$$(\boldsymbol{P}, \mathbf{t}) = (\boldsymbol{P}, \mathbf{t}_i + \mathbf{t}_l) = \left[\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}, \begin{pmatrix} -\frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix} + \begin{pmatrix} \frac{1}{3} \\ \frac{1}{6} \\ \frac{1}{6} \end{pmatrix}\right], \qquad (1.4.2.7)$$

where $\mathbf{t}_i$ and $\mathbf{t}_l$ are the intrinsic and location-dependent components of the translation part $\mathbf{t}$, and are parallel and perpendicular, respectively, to the threefold axis of rotation represented by the matrix $\boldsymbol{P}$ in (1.4.2.7) (*IT* A, 1983; Shmueli, 1984). This is clearly a threefold screw axis, parallel to $[\bar{1}\bar{1}1]$. The reciprocal-lattice vectors which remain unchanged, when postmultiplied by $\boldsymbol{P}$ (or premultiplied by its transpose), have the form: $\mathbf{h}^T = (h\bar{h}\bar{h})$; this is the special position for the present example. We see that (i) $\mathbf{h}^T\mathbf{t}_l = 0$, as expected, and (ii) $\mathbf{h}^T\mathbf{t}_i = -h$. Since the scalar product $\mathbf{h}^T\mathbf{t}$ is an integer, there are no values of index h for which the structure factor $F(h\bar{h}\bar{h})$ must be absent.

Other approaches to systematically absent reflections include a direct inspection of the structure-factor equation (Lipson & Cochran, 1966), which is of considerable didactical value, and the utilization of transformation properties of direct and reciprocal base vectors and lattice-point coordinates (Buerger, 1942).

Finally, the relationship between the phases of symmetry-related reflections, given by (1.4.2.5), is of fundamental as well as practical importance in the theories and techniques of crystal structure determination which operate in reciprocal space (Part 2 of this volume).

1.4.2.3. *Symmetry factors for space-group-specific Fourier summations*

The weighted reciprocal lattice, with weights taken as the structure factors, is synonymous with the discrete space of the coefficients of a Fourier expansion of the electron density, or the Fourier space (F space) of the latter. Accordingly, the asymmetric unit of the Fourier space can be defined as the subset of structure factors within which the relationship (1.4.2.3) does not hold – except at special positions in the reciprocal lattice. If the point group of the crystal is of order g, this is also the order of the corresponding factor-group representation of the space group (*IT* A, 1983) and there exist g relationships of the form of (1.4.2.3):

$$F(\boldsymbol{P}_s^T\mathbf{h}) = F(\mathbf{h})\exp(-2\pi i\mathbf{h}^T\mathbf{t}_s). \qquad (1.4.2.8)$$

We can thus decompose the summation in (1.4.2.1) into g sums, each extending over an asymmetric unit of the F space. It must be kept in mind, however, that some classes of reciprocal-lattice vectors may be common to more than one asymmetric unit, and thus each reciprocal-lattice point will be assigned an occupancy factor, denoted by $q(\mathbf{h})$, such that $q(\mathbf{h}) = 1$ for a general position and $q(\mathbf{h}) = 1/m(\mathbf{h})$ for a special one, where $m(\mathbf{h})$ is the multiplicity – or the order of the point group that leaves $\mathbf{h}$ unchanged. Equation (1.4.2.1) can now be rewritten as

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{s=1}^{g}\sum_{\mathbf{h}_a} q(\mathbf{h}_a)F(\boldsymbol{P}_s^T\mathbf{h}_a)\exp[-2\pi i(\boldsymbol{P}_s^T\mathbf{h}_a)^T\mathbf{r}], \qquad (1.4.2.9)$$

where the inner summation in (1.4.2.9) extends over the reference asymmetric unit of the Fourier space, which is associated with the identity operation of the space group. Substituting from (1.4.2.8) for $F(\boldsymbol{P}_s^T\mathbf{h}_a)$, and interchanging the order of the summations in (1.4.2.9), we obtain

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{h}_a} q(\mathbf{h}_a)F(\mathbf{h}_a)\sum_{s=1}^{g}\exp[-2\pi i\mathbf{h}_s^T(\boldsymbol{P}_s\mathbf{r} + \mathbf{t}_s)] \qquad (1.4.2.10)$$

$$= \frac{1}{V}\sum_{\mathbf{h}_a} q(\mathbf{h}_a)F(\mathbf{h}_a)[A(\mathbf{h}_a) - iB(\mathbf{h}_a)], \qquad (1.4.2.11)$$

where

$$A(\mathbf{h}) = \sum_{s=1}^{g}\cos[2\pi\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r} + \mathbf{t}_s)] \qquad (1.4.2.12)$$

and

$$B(\mathbf{h}) = \sum_{s=1}^{g}\sin[2\pi\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r} + \mathbf{t}_s)]. \qquad (1.4.2.13)$$

The symmetry factors A and B are well known as geometric or trigonometric structure factors and a considerable part of Volume I of *IT* (1952) is dedicated to their tabulation. Their formal association with the structure factor – following from direct-space arguments – is closely related to that shown in equation (1.4.2.11) (see Section 1.4.2.4). Simplified trigonometric expressions for A and B are given in Tables A1.4.3.1–A1.4.3.7 in Appendix 1.4.3 for all the two- and three-dimensional crystallographic space groups, and for all the parities of *hkl* for which A and B assume different functional forms. These expressions are there given for general reflections and can also be used for special ones, provided the occupancy factors $q(\mathbf{h})$ have been properly accounted for.

Equation (1.4.2.11) is quite general and can, of course, be applied to noncentrosymmetric Fourier summations, without neglect of dispersion. Further simplifications are obtained in the centrosymmetric case, when the space-group origin is chosen at a centre of symmetry, and in the noncentrosymmetric case, when dispersion is neglected. In each of the latter two cases the summation over $\mathbf{h}_a$ is restricted to reciprocal-lattice vectors that are not related by real or apparent inversion (denoted by $\mathbf{h}_a > 0$), and we obtain

$$\rho(\mathbf{r}) = \frac{2}{V}\sum_{\mathbf{h}_a>0} q(\mathbf{h}_a)F(\mathbf{h}_a)A(\mathbf{h}_a) \qquad (1.4.2.14)$$

and

$$\rho(\mathbf{r}) = \frac{2}{V}\sum_{\mathbf{h}_a>0} q(\mathbf{h}_a)|F(\mathbf{h}_a)|[A(\mathbf{h}_a)\cos\varphi(\mathbf{h}_a) + B(\mathbf{h}_a)\sin\varphi(\mathbf{h}_a)] \qquad (1.4.2.15)$$

for the dispersionless centrosymmetric and noncentrosymmetric cases, respectively.

1.4.2.4. *Symmetry factors for space-group-specific structure-factor formulae*

The explicit dependence of structure-factor summations on the space-group symmetry of the crystal can also be expressed in terms of symmetry factors, in an analogous manner to that described for the electron density in the previous section. It must be pointed out that while the above treatment only presumes that the electron density can be represented by a three-dimensional Fourier series, the present one is restricted by the assumption that the atoms are isotropic with regard to their motion and shape (*cf.* Chapter 1.2).

Under the above assumptions, *i.e.* for isotropically vibrating spherical atoms, the structure factor can be written as

$$F(\mathbf{h}) = \sum_{j=1}^{N} f_j\exp(2\pi i\mathbf{h}^T\mathbf{r}_j), \qquad (1.4.2.16)$$

where $\mathbf{h}^T = (hkl)$ is the diffraction vector, N is the number of atoms in the unit cell, f_j is the atomic scattering factor including its temperature factor and depending on the magnitude of $\mathbf{h}$ only, and $\mathbf{r}_j$ is the position vector of the jth atom referred to the origin of the unit cell.

If the crystal belongs to a point group of order m_p and the multiplicity of its Bravais lattice is m_L, there are $g' = m_p \times m_L$ general equivalent positions in the unit cell of the space group (*IT* A, 1983). We can thus rewrite (1.4.2.16), grouping the contributions of the symmetry-related atoms, as

$$F(\mathbf{h}) = \sum_j f_j\sum_{s=1}^{g'}\exp[2\pi i\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r} + \mathbf{t}_s)], \qquad (1.4.2.17)$$

where $\boldsymbol{P}_s$ and $\mathbf{t}_s$ are the rotation and translation parts of the sth space-group operation respectively. The inner summation in (1.4.2.17) contains the dependence of the structure factor of reflection $\mathbf{h}$ on the space-group symmetry of the crystal and is known as the (complex) geometric or trigonometric structure factor.

Equation (1.4.2.17) can be rewritten as

$$F(\mathbf{h}) = \sum_j f_j[A_j(\mathbf{h}) + iB_j(\mathbf{h})], \qquad (1.4.2.18)$$

where

$$A_j(\mathbf{h}) = \sum_{s=1}^{g'}\cos[2\pi\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r}_j + \mathbf{t}_s)] \qquad (1.4.2.19)$$

and

$$B_j(\mathbf{h}) = \sum_{s=1}^{g'}\sin[2\pi\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r}_j + \mathbf{t}_s)] \qquad (1.4.2.20)$$

are the real and imaginary parts of the trigonometric structure factor. Equations (1.4.2.19) and (1.4.2.20) are *mathematically* identical to equations (1.4.2.11) and (1.4.2.12), respectively, apart from the numerical coefficients which appear in the expressions for A and B, for space groups with centred lattices: while only the order of the point group need be considered in connection with the Fourier expansion of the electron density (see above), the multiplicity of the Bravais lattice must of course appear in (1.4.2.19) and (1.4.2.20).

Analogous functional forms are arrived at by considerations of symmetry in direct and reciprocal spaces. These quantities are therefore convenient representations of crystallographic symmetry in its interaction with the diffraction experiment and have been indispensable in all of the early crystallographic computing related to structure determination. Their applications to modern crystallographic computing have been largely superseded by fast Fourier techniques, in reciprocal space, and by direct use of matrix and vector representations of space-group operators, in direct space, especially in cases of low space-group symmetry. It should be noted, however, that the degree of simplification of the trigonometric structure factors generally increases with increasing symmetry (see, *e.g.*, Section 1.4.3), and the gain of computing efficiency becomes significant when problems involving high symmetries are treated with this 'old-fashioned' tool. Analytic expressions for the trigonometric structure factors are of course indispensable in studies in which the knowledge of the functional form of the structure factor is required [*e.g.* in theories of structure-factor statistics and direct methods of phase determination (see Chapters 2.1 and 2.2)].

Equations (1.4.2.19) and (1.4.2.20) are simple but their expansion and simplification for all the space groups and relevant *hkl* subsets can be an extremely tedious undertaking when carried out in the conventional manner. As shown below, this process has been automated by a suitable combination of symbolic and numeric high-level programming procedures.

1.4.3. Structure-factor tables

1.4.3.1. *Some general remarks*

This section is a revised version of the structure-factor tables contained in Sections 4.5 through 4.7 of Volume I (*IT* I, 1952). As in the previous edition, it is intended to present a comprehensive list of explicit expressions for the real and the imaginary parts of the trigonometric structure factor, for all the 17 plane groups and the 230 space groups, and for the *hkl* subsets for which the trigonometric structure factor assumes different functional forms. The tables given here are also confined to the case of general Wyckoff positions (*IT* I, 1952). However, the expressions are presented in a much more concise symbolic form and are amenable to computation just like the explicit trigonometric expressions in Volume I (*IT* I, 1952). The present tabulation is based on equations (1.4.2.19) and (1.4.2.20), *i.e.* the numerical coefficients in A and B which appear in Tables A1.4.3.1–A1.4.3.7 in Appendix 1.4.3 are appropriate to space-group-specific structure-factor formulae. The functional form of A and B is, however, the same when applied to Fourier summations (see Section 1.4.2.3).

1.4.3.2. *Preparation of the structure-factor tables*

The lists of the coordinates of the general equivalent positions, presented in *IT* A (1983), as well as in earlier editions of the *Tables*, are sufficient for the expansion of the summations in (1.4.2.19) and (1.4.2.20) and the simplification of the resulting expressions can be performed using straightforward algebra and trigonometry (see, *e.g.*, *IT* I, 1952). As mentioned above, the preparation of the present structure-factor tables has been automated and its stages can be summarized as follows:

(i) Generation of the coordinates of the general positions, starting from a computer-adapted space-group symbol (Shmueli, 1984).

(ii) Formation of the scalar products, appearing in (1.4.2.19) and (1.4.2.20), and their separation into components depending on the rotation and translation parts of the space-group operations:

$$\mathbf{h}^T(\boldsymbol{P}_s, \mathbf{t}_s)\mathbf{r} = \mathbf{h}^T\boldsymbol{P}_s\mathbf{r} + \mathbf{h}^T\mathbf{t}_s \qquad (1.4.3.1)$$

for the space groups which are not associated with a unique axis; the left-hand side of (1.4.3.1) is separated into contributions of the relevant plane group and unique axis for the remaining space groups.

(iii) Analysis of the translation-dependent parts of the scalar products and automatic determination of all the parities of *hkl* for which A and B must be computed and simplified.

(iv) Expansion of equations (1.4.2.19) and (1.4.2.20) and their reduction to trigonometric expressions comparable to those given in the structure-factor tables in Volume I of *IT* (1952).

(v) Representation of the results in terms of a small number of building blocks, of which the expressions were found to be composed. These representations are described in Section 1.4.3.3.

All the stages outlined above were carried out with suitably designed computer programs, written in numerically and symbolically oriented languages. A brief summary of the underlying algorithms is presented in Appendix 1.4.1. The computer-adapted space-group symbols used in these computations are described in Section A1.4.2.2 and presented in Table A1.4.2.1.

1.4.3.3. *Symbolic representation of A and B*

We shall first discuss the symbols for the space groups that are not associated with a unique axis. These comprise the triclinic, orthorhombic and cubic space groups. The symbols are also used for the seven rhombohedral space groups which are referred to rhombohedral axes (*IT* I, 1952; *IT* A, 1983).

The abbreviation of triple products of trigonometric functions such as, *e.g.*, denoting $\cos(2\pi hx)\sin(2\pi ky)\cos(2\pi lz)$ by csc, is well known (*IT* I, 1952), and can be conveniently used in representing A and B for triclinic and orthorhombic space groups. However, the simplified expressions for A and B in space groups of higher symmetry also possess a high degree of regularity, as is apparent from an examination of the structure-factor tables in Volume I (*IT* I, 1952), and as confirmed by the preparation of the present tables. An example, illustrating this for the cubic system, is given below.

The trigonometric structure factor for the space group $Pm\bar{3}$ (No. 200) is given by

$$\begin{aligned} A = 8[&\cos(2\pi hx)\cos(2\pi ky)\cos(2\pi lz) \\ &+ \cos(2\pi hy)\cos(2\pi kz)\cos(2\pi lx) \\ &+ \cos(2\pi hz)\cos(2\pi kx)\cos(2\pi ly)], \end{aligned} \qquad (1.4.3.2)$$

and the sum of the above nine-function block and the following one:

$$\begin{aligned} 8[&\cos(2\pi hx)\cos(2\pi kz)\cos(2\pi ly) \\ &+ \cos(2\pi hz)\cos(2\pi ky)\cos(2\pi lx) \\ &+ \cos(2\pi hy)\cos(2\pi kx)\cos(2\pi lz)] \end{aligned} \qquad (1.4.3.3)$$

is the trigonometric structure factor for the space group $Pm\bar{3}m$ (No. 221, *IT* I, 1952, *IT* A, 1983). It is obvious that the only difference between the nine-function blocks in (1.4.3.2) and (1.4.3.3) is that the permutation of the coordinates *xyz* is *cyclic* or *even* in (1.4.3.2), while it is *non-cyclic* or *odd* in (1.4.3.3).

It was observed during the generation of the present tables that the expressions for A and B for all the cubic space groups, and all the relevant *hkl* subsets, can be represented in terms of such 'even' and 'odd' nine-function blocks. Moreover, it was found that the order of the trigonometric functions in each such block remains the same in each of its three terms (triple products). This is not surprising since each of the above space groups contains threefold axes of rotation along [111] and related directions, and such permutations of *xyz* for fixed *hkl* (or *vice versa*) are expected. It was therefore possible to introduce two permutation operators and represent *A* and *B* in terms of the following two basic blocks:

$$\begin{aligned}\mathrm{Epqr} &= \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky)\mathrm{r}(2\pi lz) + \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kz)\mathrm{r}(2\pi lx)\\ &\quad + \mathrm{p}(2\pi hz)\mathrm{q}(2\pi kx)\mathrm{r}(2\pi ly)\end{aligned} \qquad (1.4.3.4)$$

and

$$\begin{aligned}\mathrm{Opqr} &= \mathrm{p}(2\pi hx)\mathrm{q}(2\pi kz)\mathrm{r}(2\pi ly) + \mathrm{p}(2\pi hz)\mathrm{q}(2\pi ky)\mathrm{r}(2\pi lx)\\ &\quad + \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kx)\mathrm{r}(2\pi lz),\end{aligned} \qquad (1.4.3.5)$$

where each of p, q and r can be a sine or a cosine, and appears at the same position in each of the three terms of a block. The capital prefixes E and O were chosen to represent even and odd permutations of the coordinates *xyz*, respectively.

For example, the trigonometric structure factor for the space group $Pa\bar{3}$ (No. 205, *IT* I, 1952, *IT* A, 1983) can now be tabulated as follows:

A	B	$h+k$	$k+l$	$h+l$
8Eccc	0	even	even	even
− 8Ecss	0	even	odd	odd
− 8Escs	0	odd	even	odd
− 8Essc	0	odd	odd	even

(*cf.* Table A1.4.3.7), where the sines and cosines are abbreviated by s and c, respectively. It is interesting to note that the only maximal non-isomorphic subgroup of $Pa\bar{3}$, not containing a threefold axis, is the orthorhombic *Pbca* (see *IT* A, 1983, p. 621), and this group–subgroup relationship is reflected in the functional forms of the trigonometric structure factors; the representation of *A* and *B* for *Pbca* is in fact analogous to that of $Pa\bar{3}$, including the parities of *hkl* and the corresponding forms of the triple products, except that the prefix E – associated with the threefold rotation – is absent from *Pbca*. The expression for *A* for the space group $Pm\bar{3}m$ [the sum of (1.4.3.2) and (1.4.3.3)] now simply reads: $A = 8(\mathrm{Eccc} + \mathrm{Occc})$.

As pointed out above, the permutation operators also apply to rhombohedral space groups that are referred to rhombohedral axes (Table A1.4.3.6), and the corresponding expressions for $R3$ and $R\bar{3}$ bear the same relationship to those for $P1$ and $P\bar{1}$ (Table A1.4.3.2), respectively, as that shown above for the related $Pa\bar{3}$ and *Pbca*.

When in any given standard space-group setting one of the coordinate axes is parallel to a unique axis, the point-group rotation matrices can be partitioned into 2×2 and 1×1 diagonal blocks, the former corresponding to an operation of the plane group resulting from the projection of the space group down the unique axis. If, for example, the unique axis is parallel to **c**, we can decompose the scalar product in (1.4.2.19) and (1.4.2.20) as follows:

$$\begin{aligned}\mathbf{h}^T(\boldsymbol{P}_s\mathbf{r}+\mathbf{t}_s) &= (\,h \quad k\,)\left[\begin{pmatrix} P_{11} & P_{12}\\ P_{21} & P_{22}\end{pmatrix}\begin{pmatrix} x\\ y\end{pmatrix} + \begin{pmatrix} t_1\\ t_2\end{pmatrix}\right]\\ &\quad + l(P_{33}z + t_3),\end{aligned} \qquad (1.4.3.6)$$

where the first scalar product on the right-hand side of (1.4.3.6) contains the contribution of a plane group and the second product is the contribution of the unique axis itself. The above decomposition often leads to a convenient factorization of *A* and *B*, and is applicable to monoclinic, tetragonal and hexagonal families, the latter including rhombohedral space groups that are referred to hexagonal axes.

The symbols used in Tables A1.4.3.3, A1.4.3.5 and A1.4.3.6 are based on such decompositions. In those few cases where explicit expressions must be given we make use of the convention of replacing $\cos(2\pi u)$ by $\mathrm{c}(u)$ and $\sin(2\pi u)$ by $\mathrm{s}(u)$. For example, $\cos[2\pi(hy+kx)]$ *etc.* is given as $\mathrm{c}(hy+kx)$ *etc.* The symbols are defined below.

Monoclinic space groups (Table A1.4.3.3)

The following symbols are used in this system:

$$\begin{aligned}\mathrm{c}(hl) &= \cos[2\pi(hx+lz)], \quad \mathrm{c}(hk) = \cos[2\pi(hx+ky)]\\ \mathrm{s}(hl) &= \sin[2\pi(hx+lz)], \quad \mathrm{s}(hk) = \sin[2\pi(hx+ky)]\end{aligned} \qquad (1.4.3.7)$$

so that any expression for *A* or *B* in the monoclinic system has the form $K\mathrm{p}(hl)\mathrm{q}(ky)$ or $K\mathrm{p}(hk)\mathrm{q}(lz)$ for the second or first setting, respectively, where p and q can each be a sine or a cosine and *K* is a numerical constant.

Tetragonal space groups (Table A1.4.3.5)

The most frequently occurring expressions in the summations for *A* and *B* in this system are of the form

$$\mathrm{P(pq)} = \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) + \mathrm{p}(2\pi kx)\mathrm{q}(2\pi hy) \qquad (1.4.3.8)$$

and

$$\mathrm{M(pq)} = \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) - \mathrm{p}(2\pi kx)\mathrm{q}(2\pi hy), \qquad (1.4.3.9)$$

where p and q can each be a sine or a cosine. These are typical contributions related to square plane groups.

Trigonal and hexagonal space groups (Table A1.4.3.6)

The contributions of plane hexagonal space groups to the first term in (1.4.3.6) are

$$\begin{aligned} p_1 &= hx+ky, \quad p_2 = kx+iy, \quad p_3 = ix+hy,\\ q_1 &= kx+hy, \quad q_2 = hx+iy, \quad q_3 = ix+ky,\end{aligned} \qquad (1.4.3.10)$$

where $i = -h-k$ (*IT* I, 1952). The symbols which represent the frequently occurring expressions in this family, and given in terms of (1.4.3.10), are

$$\begin{aligned}\mathrm{C}(hki) &= \cos(2\pi p_1) + \cos(2\pi p_2) + \cos(2\pi p_3)\\ \mathrm{C}(khi) &= \cos(2\pi q_1) + \cos(2\pi q_2) + \cos(2\pi q_3)\\ \mathrm{S}(hki) &= \sin(2\pi p_1) + \sin(2\pi p_2) + \sin(2\pi p_3)\\ \mathrm{S}(khi) &= \sin(2\pi q_1) + \sin(2\pi q_2) + \sin(2\pi q_3)\end{aligned} \qquad (1.4.3.11)$$

and these quite often appear as the following sums and differences:

$$\begin{aligned}\mathrm{PH(cc)} &= \mathrm{C}(hki) + \mathrm{C}(khi), \quad \mathrm{PH(ss)} = \mathrm{S}(hki) + \mathrm{S}(khi)\\ \mathrm{MH(cc)} &= \mathrm{C}(hki) - \mathrm{C}(khi), \quad \mathrm{MH(ss)} = \mathrm{S}(hki) - \mathrm{S}(khi).\end{aligned} \qquad (1.4.3.12)$$

The symbols defined in this section are briefly redefined in the appropriate tables, which also contain the conditions for vanishing symbols.

1.4.3.4. *Arrangement of the tables*

The expressions for *A* and *B* are usually presented in terms of the short symbols defined above for all the representations of the plane groups and space groups given in Volume A (*IT* A, 1983), and are fully consistent with the unit-cell choices and space-group origins employed in that volume. The tables are arranged by crystal families and the expressions appear in the order of the appearance of the corresponding plane and space groups in the space-group tables in *IT* A (1983).

The main items in a table entry, not necessarily in the following order, are: (i) the conventional space-group number, (ii) the short Hermann–Mauguin space-group symbol, (iii) brief remarks on the choice of the space-group origin and setting, where appropriate, (iv) the real (*A*) and imaginary (*B*) parts of the trigonometric structure factor, and (v) the parity of the *hkl* subset to which the expressions for A and B pertain. Full space-group symbols are given in the monoclinic system only, since they are indispensable for the recognition of the settings and glide planes appearing in the various representations of monoclinic space groups given in *IT* A (1983).

1.4.4. Symmetry in reciprocal space: space-group tables

1.4.4.1. *Introduction*

The purpose of this section, and the accompanying table, is to provide a representation of the 230 three-dimensional crystallographic space groups in terms of two fundamental quantities that characterize a weighted reciprocal lattice: (i) coordinates of point-symmetry-related points in the reciprocal lattice, and (ii) phase shifts of the weight functions that are associated with the translation parts of the various space-group operations. Table A1.4.4.1 in Appendix 1.4.4 collects the above information for all the space-group settings which are listed in *IT* A (1983) for the same choice of the space-group origins and following the same numbering scheme used in that volume. Table A1.4.4.1 was generated by computer using the space-group algorithm described by Shmueli (1984) and the space-group symbols given in Table A1.4.2.1 in Appendix 1.4.2. It is shown in a later part of this section that Table A1.4.4.1 can also be regarded as a table of symmetry groups in Fourier space, in the Bienenstock–Ewald (1962) sense which was mentioned in Section 1.4.1. The section is concluded with a brief description of the correspondence between Bravais-lattice types in direct and reciprocal spaces.

1.4.4.2. *Arrangement of the space-group tables*

Table A1.4.4.1 is subdivided into point-group sections and space-group subsections, as outlined below.

(i) *The point-group heading.* This heading contains a short Hermann–Mauguin symbol of a point group, the crystal system and the symbol of the Laue group with which the point group is associated. Each point-group heading is followed by the set of space groups which are isomorphic to the point group indicated, the set being enclosed within a box.

(ii) *The space-group heading.* This heading contains, for each space group listed in Volume A (*IT* A, 1983), the short Hermann–Mauguin symbol of the space group, its conventional space-group number and (in parentheses) the serial number of its representation in Volume A; this is also the serial number of the explicit space-group symbol in Table A1.4.2.1 from which the entry was derived. Additional items are full space-group symbols, given only for the monoclinic space groups in their settings that are given in Volume A (*IT*, 1983), and self-explanatory comments as required.

(iii) *The table entry.* In the context of the analysis in Section 1.4.2.2, the format of a table entry is: $\mathbf{h}^T\boldsymbol{P}_n : -\mathbf{h}^T\mathbf{t}_n$, where $(\boldsymbol{P}_n, \mathbf{t}_n)$ is the nth space-group operator, and the phase shift $\mathbf{h}^T\mathbf{t}_n$ is expressed in units of 2π [see equations (1.4.2.3) and (1.4.2.5)]. More explicitly, the general format of a table entry is

$$(n)\ h_nk_nl_n : -p_nq_nr_n/m. \qquad (1.4.4.1)$$

In (1.4.4.1), n is the serial number of the space-group operation to which this entry pertains and is the same as the number of the general Wyckoff position generated by this operation and given in *IT* A (1983) for the space group appearing in the space-group heading. The first part of an entry, $h_nk_nl_n$:, contains the coordinates of the reciprocal-lattice vector that was generated from the reference vector (*hkl*) by the rotation part of the nth space-group operation. These rotation parts of the table entries, for a given space group, thus constitute the set of reciprocal-lattice points that are generated by the corresponding point group (*not Laue group*). The second part of an entry is an abbreviation of the phase shift which is associated with the nth operation and thus

$$-p_nq_nr_n/m \quad \text{denotes} \quad -2\pi(hp_n + kq_n + lr_n)/m, \qquad (1.4.4.2)$$

where the fractions $p_n/m, q_n/m$ and r_n/m are the components of the translation part $\mathbf{t}_n$ of the nth space-group operation. The phase-shift part of an entry is given only if $(p_nq_nr_n)$ is *not* a vector in the direct lattice, since such a vector would give rise to a trivial phase shift (an integer multiple of 2π).

1.4.4.3. *Effect of direct-space transformations*

The phase shifts given in Table A1.4.4.1 depend on the translation parts of the space-group operations and these translations are determined, all or in part, by the choice of the space-group origin. It is a fairly easy matter to find the phase shifts that correspond to a given shift of the space-group origin in direct space, directly from Table A1.4.4.1. Moreover, it is also possible to modify the table entries so that a more general transformation, including a change of crystal axes as well as a shift of the space-group origin, can be directly accounted for. We employ here the frequently used concise notation due to Seitz (1935) (see also *IT* A, 1983).

Let the direct-space transformation be given by

$$\mathbf{r}_{\rm new} = \boldsymbol{T}\mathbf{r}_{\rm old} + \mathbf{v}, \qquad (1.4.4.3)$$

where $\boldsymbol{T}$ is a non-singular 3×3 matrix describing the change of the coordinate system and $\mathbf{v}$ is an origin-shift vector. The components of $\boldsymbol{T}$ and $\mathbf{v}$ are referred to the old system, and $\mathbf{r}_{\rm new}$ $(\mathbf{r}_{\rm old})$ is the position vector of a point in the crystal, referred to the new (old) system, respectively. If we denote a space-group operation referred to the new and old systems by $(\boldsymbol{P}_{\rm new}, \mathbf{t}_{\rm new})$ and $(\boldsymbol{P}_{\rm old}, \mathbf{t}_{\rm old})$, respectively, we have

$$(\boldsymbol{P}_{\rm new}, \mathbf{t}_{\rm new}) = (\boldsymbol{T}, \mathbf{v})(\boldsymbol{P}_{\rm old}, \mathbf{t}_{\rm old})(\boldsymbol{T}, \mathbf{v})^{-1} \qquad (1.4.4.4)$$

$$= (\boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}, \mathbf{v} - \boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}\mathbf{v} + \boldsymbol{T}\mathbf{t}_{\rm old}). \qquad (1.4.4.5)$$

It follows from (1.4.4.2) and (1.4.4.5) that if the old entry of Table A1.4.4.1 is given by

$$(n)\ \mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t},$$

the transformed entry becomes

$$(n)\ \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1} : \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1}\mathbf{v} - \mathbf{h}^T\mathbf{v} - \mathbf{h}^T\boldsymbol{T}\mathbf{t}, \qquad (1.4.4.6)$$

and in the important special cases of a pure change of setting ($\mathbf{v} = 0$) or a pure shift of the space-group origin ($\boldsymbol{T}$ is the unit matrix $\boldsymbol{I}$), (1.4.4.6) reduces to

$$(n)\ \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1} : -\mathbf{h}^T\boldsymbol{T}\mathbf{t} \qquad (1.4.4.7)$$

or

$$(n)\ \mathbf{h}^T\boldsymbol{P} : \mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{v} - \mathbf{h}^T\mathbf{t}, \qquad (1.4.4.8)$$

respectively. The rotation matrices $\boldsymbol{P}$ are readily obtained by visual or programmed inspection of the old entries: if, for example, $\mathbf{h}^T\boldsymbol{P}$ is *khl*, we must have $P_{21} = 1$, $P_{12} = 1$ and $P_{33} = 1$, the remaining P_{ij}'s being equal to zero. Similarly, if $\mathbf{h}^T\boldsymbol{P}$ is *kil*, where $i = -h - k$, we have

$$(kil) = (k, -h-k, l) = (hkl)\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The rotation matrices can also be obtained by reference to Chapter 7 and Tables 11.2 and 11.3 in Volume A (*IT* A, 1983).

As an example, consider the phase shifts corresponding to the operation No. (16) of the space group $P4/nmm$ (No. 129) in its two origins given in Volume A (*IT* A, 1983). For an Origin 2-to-Origin 1 transformation we find there $\mathbf{v} = (\frac{1}{4}, -\frac{1}{4}, 0)$ and the old Origin 2 entry in Table A1.4.4.1 is (16) *khl* (**t** is zero). The appropriate entry for the Origin 1 description of this operation should therefore be $\mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{v} = k/4 - h/4 - h/4 + k/4 = -h/2 + k/2$, as given by (1.4.4.8), or $-(h+k)/2$ if a trivial shift of 2π is subtracted. The (new) Origin 1 entry thus becomes: (16) *khl*: $-110/2$, as listed in Table A1.4.4.1.

1.4.4.4. *Symmetry in Fourier space*

As shown below, Table A1.4.4.1 can also be regarded as a collection of the general equivalent positions of the symmetry groups of Fourier space, in the sense of the treatment by Bienenstock & Ewald (1962). This interpretation of the table is, however, restricted to the underlying periodic function being real and positive (see the latter reference). The symmetry formalism can be treated with the aid of the original 4×4 matrix notation, but it appears that a concise Seitz-type notation suits better the present introductory interpretation.

The symmetry dependence of the fundamental relationship (1.4.2.5)

$$\varphi(\mathbf{h}^T\boldsymbol{P}_n) = \varphi(\mathbf{h}) - 2\pi\mathbf{h}^T\mathbf{t}_n$$

is given by a table entry of the form: $(n)\ \mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}$, where the phase shift is given in units of 2π, and the structure-dependent phase $\varphi(\mathbf{h})$ is omitted. Defining a combination law analogous to Seitz's product of two operators of affine transformation:

$$[\mathbf{a}^T : b](\boldsymbol{R}, \mathbf{r}) = [\mathbf{a}^T\boldsymbol{R} : \mathbf{a}^T\mathbf{r} + b], \tag{1.4.4.9}$$

where $\boldsymbol{R}$ is a 3×3 matrix, $\mathbf{a}^T$ is a row vector, $\mathbf{r}$ is a column vector and b is a scalar, we can write the general form of a table entry as

$$[\mathbf{h}^T : \delta](\boldsymbol{P}, -\mathbf{t}) = [\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t} + \delta], \tag{1.4.4.10}$$

where δ is a constant phase shift which we take as zero. The positions $[\mathbf{h}^T : 0]$ and $[\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}]$ are now related by the operation $(\boldsymbol{P}, -\mathbf{t})$ *via* the combination law (1.4.4.9), which is a shorthand transcription of the 4×4 matrix notation of Bienenstock & Ewald (1962), with the appropriate sign of **t**.

Let us evaluate the result of a successive application of two such operators, say $(\boldsymbol{P}, -\mathbf{t})$ and $(\boldsymbol{Q}, -\mathbf{v})$ to the reference position $[\mathbf{h}^T : 0]$ in Fourier space:

$$\begin{aligned}[\mathbf{h}^T : 0](\boldsymbol{P}, -\mathbf{t})(\boldsymbol{Q}, -\mathbf{v}) &= [\mathbf{h}^T : 0](\boldsymbol{PQ}, -\boldsymbol{P}\mathbf{v} - \mathbf{t})\\ &= [\mathbf{h}^T\boldsymbol{PQ} : -\mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{t}],\end{aligned} \tag{1.4.4.11}$$

and perform an inverse operation:

$$\begin{aligned}[\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}](\boldsymbol{P}, -\mathbf{t})^{-1} &= [\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}](\boldsymbol{P}^{-1}, \boldsymbol{P}^{-1}\mathbf{t})\\ &= [\mathbf{h}^T\boldsymbol{PP}^{-1} : \mathbf{h}^T\boldsymbol{PP}^{-1}\mathbf{t} - \mathbf{h}^T\mathbf{t}]\\ &= [\mathbf{h}^T : 0].\end{aligned} \tag{1.4.4.12}$$

These equations confirm the validity of the shorthand notation (1.4.4.9) and illustrate the group nature of the operators $(\boldsymbol{P}, -\mathbf{t})$ in the present context.

Following Bienenstock & Ewald, the operators $(\boldsymbol{P}, -\mathbf{t})$ are symmetry operators that act on the positions $[\mathbf{h}^T : 0]$ in Fourier space, provided they satisfy the following requirements: (i) the application of such an operator leaves the magnitude of the (generally) complex Fourier coefficient unchanged, and (ii) after g successive applications of an operator, where g is the order of its rotation part, the phase remains unchanged up to a shift by an integer multiple of 2π (a trivial phase shift, corresponding to a translation by a lattice vector in direct space).

If our function is the electron density in the crystal, the first requirement is obviously satisfied since $|F(\mathbf{h})| = |F(\mathbf{h}^T\boldsymbol{P})|$, where F is the structure factor [*cf.* equation (1.4.2.4)]. In order to make use of the second requirement in deriving permissible symmetry operators on Fourier space, all the relevant transformations, *i.e.* those which have rotation operators of the orders 1, 2, 3, 4 and 6, must be individually examined. A comprehensive example, covering most of the tetragonal system, can be found in Bienenstock & Ewald (1962).

It is of interest to illustrate the above process for a simple particular instance. Consider an operation, the rotation part of which involves a mirror plane, and assume that it is associated with the monoclinic system, in the second setting (unique axis b). We denote the operator by $(\boldsymbol{m}, -\mathbf{u})$, where $\mathbf{u}^T = (uvw)$, and the permissible values of u, v and w are to be determined. The operation is of order 2, and according to requirement (ii) above we have to evaluate

$$\begin{aligned}[\mathbf{h}^T : 0](\boldsymbol{m}, -\mathbf{u})^2 &= [\mathbf{h}^T : 0](\boldsymbol{I}, -\boldsymbol{m}\mathbf{u} - \mathbf{u})\\ &= [\mathbf{h}^T : -\mathbf{h}^T(\boldsymbol{m} + \boldsymbol{I})\mathbf{u}]\\ &= [hkl : -2(hu + lw)],\end{aligned} \tag{1.4.4.13}$$

where

$$\boldsymbol{m} = \begin{pmatrix} 1 & 0 & 0\\ 0 & \bar{1} & 0\\ 0 & 0 & 1 \end{pmatrix}$$

is the matrix representing the operation of reflection and $\boldsymbol{I}$ is the unit matrix. For $(\boldsymbol{m}, -\mathbf{u})$ to be an admissible symmetry operator, the phase-shift part of (1.4.4.13), *i.e.* $-2(hu + lw)$, must be an integer (multiple of 2π). The smallest non-negative values of u and w which satisfy this are the pairs: $u = w = 0$, $u = \frac{1}{2}$ and $w = 0$, $u = 0$ and $w = \frac{1}{2}$, and $u = w = \frac{1}{2}$. We have thus obtained four symmetry operators in Fourier space, which are identical (except for the sign of their translational parts) to those of the direct-space monoclinic mirror and glide-plane operations. The fact that the component v cancels out simply means that an arbitrary component of the phase shift can be added along the b^* axis; this is concurrent with arbitrary direct-space translations that appear in the characterization of individual types of space-group operations [see *e.g.* Koch & Fischer (1983)].

Each of the 230 space groups, which leaves invariant a (real and non-negative) function with the periodicity of the crystal, thus has its counterpart which determines the symmetry of the Fourier expansion coefficients of this function, with equivalent positions given in Table A1.4.4.1.

1.4.4.5. *Relationships between direct and reciprocal Bravais lattices*

Centred Bravais lattices in crystal space give rise to systematic absences of certain classes of reflections (*IT* I, 1952; *IT* A, 1983) and the corresponding points in the reciprocal lattice have accordingly zero weights. These absences are periodic in reciprocal space and their 'removal' from the reciprocal lattice results in a lattice which – like the direct one – must belong to one of the fourteen Bravais lattice types. This must be so since the point group of a crystal leaves its lattice – and also the associated reciprocal lattice – unchanged. The magnitudes of the structure factors (the weight functions) are also invariant under the operation of this point group.

The correspondence between the types of centring in direct and reciprocal lattices is given in Table 1.4.4.1.

Notes:

(i) The vectors $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$, appearing in the definition of the multiple unit cell in the reciprocal lattice, define this lattice *prior to*

Table 1.4.4.1. *Correspondence between types of centring in direct and reciprocal lattices*

Direct lattice		Reciprocal lattice		
Lattice type(s)	Centring translations	Lattice type(s)	Restriction on *hkl*	Multiple unit cell
P, R		P, R		$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$
A	$0, \frac{1}{2}, \frac{1}{2}$	A	$k + l = 2n$	$\mathbf{a}^*, 2\mathbf{b}^*, 2\mathbf{c}^*$
B	$\frac{1}{2}, 0, \frac{1}{2}$	B	$h + l = 2n$	$2\mathbf{a}^*, \mathbf{b}^*, 2\mathbf{c}^*$
C	$\frac{1}{2}, \frac{1}{2}, 0$	C	$h + k = 2n$	$2\mathbf{a}^*, 2\mathbf{b}^*, \mathbf{c}^*$
I	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	F	$h + k + l = 2n$	$2\mathbf{a}^*, 2\mathbf{b}^*, 2\mathbf{c}^*$
F	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	I	$k + l = 2n$ $h + l = 2n$ $h + k = 2n$	$2\mathbf{a}^*, 2\mathbf{b}^*, 2\mathbf{c}^*$
$R_{\rm hex}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$	$R_{\rm hex}$	$-h + k + l = 3n$	$3\mathbf{a}^*, 3\mathbf{b}^*, 3\mathbf{c}^*$

the removal of lattice points with zero weights (absences). All the restrictions on *hkl* pertain to indexing on $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$.

(ii) The centring type of the reciprocal lattice refers to the multiple unit cell given in the table.

(iii) The centring type denoted by $R_{\rm hex}$ is a representation of the rhombohedral lattice R by a triple hexagonal unit cell, in the obverse setting (*IT* I, 1952), *i.e.* according to the transformation

$$\begin{aligned} \mathbf{a} &= \mathbf{a}_R - \mathbf{b}_R \\ \mathbf{b} &= \mathbf{b}_R - \mathbf{c}_R \\ \mathbf{c} &= \mathbf{a}_R + \mathbf{b}_R + \mathbf{c}_R, \end{aligned} \qquad (1.4.4.14)$$

where $\mathbf{a}_R$, $\mathbf{b}_R$ and $\mathbf{c}_R$ pertain to a primitive unit cell in the rhombohedral lattice R.

The corresponding multiple reciprocal cell, with centring denoted by $R_{\rm hex}$, contains nine lattice points with coordinates 000, 021, 012, 101, 202, 110, 220, 211 and 122 – indexed on the usual reciprocal to the triple hexagonal unit cell defined by (1.4.4.14). Detailed derivations of these correspondences are given by Buerger (1942), and an elementary proof of the reciprocity of I and F lattices can be found, *e.g.*, in pamphlet No. 4 of the Commission on Crystallographic Teaching (Authier, 1981). Intuitive proofs follow directly from the restrictions on *hkl*, given in Table 1.4.4.1.

Appendix 1.4.1.

Comments on the preparation and usage of the tables

(U. Shmueli)

The straightforward but rather extensive calculations and text processing related to Tables A1.4.3.1 through A1.4.3.7 and Table A1.4.4.1 in Appendices 1.4.3 and 1.4.4, respectively, were performed with the aid of a combination of FORTRAN and REDUCE (Hearn, 1973) programs, designed so as to enable the author to produce the table entries directly from a space-group symbol and with a minimum amount of intermediate manual intervention. The first stage of the calculation, the generation of a space group (coordinates of the equivalent positions), was accomplished with the program *SPGRGEN*, the algorithm of which was described in some detail elsewhere (Shmueli, 1984). A complete list of computer-adapted space-group symbols, processed by *SPGRGEN* and not given in the latter reference, is presented in Table A1.4.2.1 of Appendix 1.4.2.

The generation of the space group is followed by a construction of symbolic expressions for the scalar products $\mathbf{h}^T(\boldsymbol{P}\mathbf{r} + \mathbf{t})$; *e.g.* for position No. (13) in the space group $P4_132$ (No. 213, *IT* I, 1952, *IT* A, 1983), this scalar product is given by $h(\frac{3}{4} + y) + k(\frac{1}{4} + x) + l(\frac{1}{4} - z)$. The construction of the various table entries consists of expanding the sines and cosines of these scalar products, performing the required summations, and simplifying the result where possible. The construction of the scalar products in a FORTRAN program is fairly easy and the extremely tedious trigonometric calculations required by equations (1.4.2.19) and (1.4.2.20) can be readily performed with the aid of one of several available computer-algebraic languages (for a review, see *Computers in the New Laboratory – a Nature Survey*, 1981); the REDUCE language was employed for the above purpose.

Since the REDUCE programs required for the summations in (1.4.2.19) and (1.4.2.20) for the various space groups were seen to have much in common, it was decided to construct a FORTRAN interface which would process the space-group input and prepare automatically REDUCE programs for the algebraic work. The least straightforward problem encountered during this work was the need to 'convince' the interface to generate *hkl* parity assignments which are appropriate to the space-group information input. This was solved for all the crystal families except the hexagonal by setting up a 'basis' of the form: $h/2, k/2, l/2, (k+l)/2, \ldots, (h+k+l)/4$ and representing the translation parts of the scalar products, $\mathbf{h}^T\mathbf{t}$, as sums of such 'basis functions'. A subsequent construction of an automatic parity routine proved to be easy and the interface could thus produce any number of REDUCE programs for the summations in (1.4.2.19) and (1.4.2.20) using a list of space-group symbols as the sole input. These included trigonal and hexagonal space groups with translation components of $\frac{1}{2}$. This approach seemed to be too awkward for some space groups containing threefold and sixfold screw axes, and these were treated individually.

There is little to say about the REDUCE programs, except that the output they generate is at the same level of trigonometric complexity as the expressions for A and B appearing in Volume I (*IT* I, 1952). This could have been improved by making use of the pattern-matching capabilities that are incorporated in REDUCE, but it was found more convenient to construct a FORTRAN interpreter which would detect in the REDUCE output the basic building blocks of the trigonometric structure factors (see Section 1.4.3.3) and perform the required transformations.

Tables A1.4.3.1–A1.4.3.7 were thus constructed with the aid of a chain composed of (i) a space-group generating routine, (ii) a FORTRAN interface, which processes the space-group input and 'writes' a complete REDUCE program, (iii) execution of the REDUCE program and (iv) a FORTRAN interpreter of the REDUCE output in terms of the abbreviated symbols to be used in the tables. The computation was at a 'one-group-at-a-time' basis and the automation of its repetition was performed by means of procedural constructs at the operating-system level. The construction of Table A1.4.4.1 involved only the preliminary stage of the processing of the space-group information by the FORTRAN interface. All the computations were carried out on a Cyber 170-855 at the Tel Aviv University Computation Center.

It is of some importance to comment on the recommended usage of the tables included in this chapter in automatic computations. If, for example, we wish to compute the expression: $A = -8(\text{Escs} + \text{Ossc})$, use can be made of the facility provided by most versions of FORTRAN of transferring subprogram names as parameters of a FUNCTION. We thus need only two FUNCTIONs for any calculation of A and B for a cubic space group, one FUNCTION for the block of even permutations of x, y and z:

```
      FUNCTION E(P, Q, R)
      EXTERNAL SIN, COS
      COMMON/TSF/TPH, TPK, TPL, X, Y, Z
      E = P(TPH * X) * Q(TPK * Y) * R(TPL * Z)
    1 + P(TPH * Z) * Q(TPK * X) * R(TPL * Y)
    2 + P(TPH * Y) * Q(TPK * Z) * R(TPL * X)
      RETURN
      END
```

where TPH, TPK and TPL denote $2\pi h$, $2\pi k$ and $2\pi l$, respectively, and a similar FUNCTION, say O(P,Q,R), for the block of odd permutations of x, y and z. The calling statement in the calling (sub)program can thus be:

```
A = -8 * (E(SIN, COS, SIN) + O(SIN, SIN, COS)).
```

A small number of such FUNCTIONs suffices for all the space-group-specific computations that involve trigonometric structure factors.

Appendix 1.4.2.

Space-group symbols for numeric and symbolic computations

A1.4.2.1. *Introduction* (U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve)

This appendix lists two sets of computer-adapted space-group symbols which are implemented in existing crystallographic software and can be employed in the automated generation of space-group representations. The computer generation of space-group symmetry information is of well known importance in many crystallographic calculations, numeric as well as symbolic. A prerequisite for a computer program that generates this information is a set of computer-adapted space-group symbols which are based on the generating elements of the space group to be derived. The sets of symbols to be presented are:

(i) *Explicit symbols*. These symbols are based on the classification of crystallographic point groups and space groups by Zachariasen (1945). These symbols are termed *explicit* because they contain in an explicit manner the rotation and translation parts of the space-group generators of the space group to be derived and used. These computer-adapted explicit symbols were proposed by Shmueli (1984), who also describes in detail their implementation in the program *SPGRGEN*. This program was used for the automatic preparation of the structure-factor tables for the 17 plane groups and 230 space groups, listed in Appendix 1.4.3, and the 230 space groups in reciprocal space, listed in Appendix 1.4.4. The explicit symbols presented in this appendix are adapted to the 306 representations of the 230 space groups as presented in *IT* A (1983) with regard to the standard settings and choice of space-group origins.

The symmetry-generating algorithm underlying the explicit symbols, and their definition, are given in Section A1.4.2.2 of this appendix and the explicit symbols are listed in Table A1.4.2.1.

(ii) *Hall symbols*. These symbols are based on the implied-origin notation of Hall (1981*a*,*b*), who also describes in detail the algorithm implemented in the program *SGNAME* (Hall, 1981*a*). In the first edition of *IT* B (1993), the term 'concise space-group symbols' was used for this notation. In recent years, however, the term 'Hall symbols' has come into use in symmetry papers (Altermatt & Brown, 1987; Grosse-Kunstleve, 1999), software applications (Hovmöller, 1992; Grosse-Kunstleve, 1995; Larine *et al.*, 1995; Dowty, 1997) and data-handling approaches (Bourne *et al.*, 1998). This term has therefore been adopted for the second edition.

The main difference in the definition of the Hall symbols between this edition and the first edition of *IT* B is the generalization of the origin-shift vector to a full change-of-basis matrix. The examples have been expanded to show how this matrix is applied. The notation has also been made more consistent, and a typographical error in a default axis direction has been corrected.* The lattice centring symbol 'H' has been added to Table A1.4.2.2. In addition, Hall symbols are now provided for 530 settings to include all settings from Table 4.3.1 of *IT* A (1983). Namely, all non-standard symbols for the monoclinic and orthorhombic space groups are included.

Some of the space-group symbols listed in Table A1.4.2.7 differ from those listed in Table B.6 (p. 119) of the first edition of *IT* B. This is because the symmetry of many space groups can be represented by more than one subset of 'generator' elements and these lead to different Hall symbols. The symbols listed in this edition have been selected after first sorting the symmetry elements into a strictly prescribed order based on the shape of their Seitz matrices, whereas those in Table B.6 were selected from symmetry elements in the order of *IT* I (1965). Software for selecting the Hall symbols listed in Table A1.4.2.7 is freely available (Hall, 1997). These symbols and their equivalents in the first edition of *IT* B will generate identical symmetry elements, but the former may be used as a reference table in a strict mapping procedure between different symmetry representations (Hall *et al.*, 2000).

The Hall symbols are defined in Section A1.4.2.3 of this appendix and are listed in Table A1.4.2.7.

* The correct default axis direction $\mathbf{a} - \mathbf{b}$ of an N preceded by 3 or 6 replaces $\mathbf{a} + \mathbf{b}$ on p. 117, right-hand column, line 4, in the first edition of *IT* B.

A1.4.2.2. *Explicit symbols* (U. Shmueli)

As shown elsewhere (Shmueli, 1984), the set of representative operators of a crystallographic space group [*i.e.* the set that is listed for each space group in the symmetry tables of *IT* A (1983) and automatically regenerated for the purpose of compiling the symmetry tables in the present chapter] may have one of the following forms:

$$\begin{aligned}&\{(\mathbf{Q},\mathbf{u})\},\\ &\{(\mathbf{Q},\mathbf{u})\}\times\{(\mathbf{R},\mathbf{v})\},\quad \text{or}\\ &\{(\mathbf{P},\mathbf{t})\}\times[\{(\mathbf{Q},\mathbf{u})\}\times\{(\mathbf{R},\mathbf{v})\}],\end{aligned}\qquad (\text{A}1.4.2.1)$$

where **P**, **Q** and **R** are point-group operators, and **t**, **u** and **v** are zero vectors or translations not belonging to the lattice-translations subgroup. Each of the forms in (A1.4.2.1), enclosed in braces, is evaluated as, *e.g.*,

$$\{(\mathbf{P},\mathbf{t})\}=\{(\mathbf{I},\mathbf{0}),(\mathbf{P},\mathbf{t}),(\mathbf{P},\mathbf{t})^2,\ldots,(\mathbf{P},\mathbf{t})^{g-1}\},\qquad (\text{A}1.4.2.2)$$

where **I** is a unit operator and g is the order of the rotation operator **P** (*i.e.* $\mathbf{P}^g = \mathbf{I}$). The representative operations of the space group are evaluated by expanding the generators into cyclic groups, as in (A1.4.2.2), and forming, as needed, ordered products of the expanded groups as indicated in (A1.4.2.1) and explained in detail in the original article (Shmueli, 1984). The rotation and translation parts of the generators (**P**, **t**), (**Q**, **u**) and (**R**, **v**) presented here were adapted to the settings and choices of origin used in the main symmetry tables of *IT* A (1983).

The general structure of a three-generator symbol, corresponding to the last line of (A1.4.2.1), as represented in Table A1.4.2.1, is

$$\mathrm{LSC\$r_1Pt_1t_2t_3\$r_2Qu_1u_2u_3\$r_3Rv_1v_2v_3},\qquad (\text{A}1.4.2.3)$$

where

L – lattice type; can be `P`, `A`, `B`, `C`, `I`, `F`, or `R`. The symbol `R` is used only for the seven rhombohedral space groups in their representations in rhombohedral and hexagonal axes [obverse setting (*IT* I, 1952)].

S – crystal system; can be `A` (triclinic), `M` (monoclinic), `O` (orthorhombic), `T` (tetragonal), `R` (trigonal), `H` (hexagonal) or `C` (cubic).

C – status of centrosymmetry; can be `C` or `N` according as the space group is centrosymmetric or noncentrosymmetric, respectively.

$ – this character is followed by six characters that define a generator of the space group.

r_i – indicator of the type of rotation that follows: r_i is `P` or `I` according as the rotation part of the ith generator is proper or improper, respectively.

P, Q, R – two-character symbols of matrix representations of the point-group rotation operators **P**, **Q** and **R**, respectively (see below).

$\mathrm{t_1t_2t_3}$, $\mathrm{u_1u_2u_3}$, $\mathrm{v_1v_2v_3}$ – components of the translation parts of the generators, given in units of $\frac{1}{12}$; *e.g.* the translation part $(0\ \frac{1}{2}\ \frac{3}{4})$ is given in Table A1.4.2.1 as 069. *An exception*: $(0\ 0\ \frac{5}{6})$ is denoted by 005 and not by 0010.

The two-character symbols for the matrices of rotation, which appear in the explicit space-group symbols in Table A1.4.2.1, are defined as follows:

$$\mathtt{1A}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\quad \mathtt{2A}=\begin{pmatrix}1&0&0\\0&\bar1&0\\0&0&\bar1\end{pmatrix}\quad \mathtt{2B}=\begin{pmatrix}\bar1&0&0\\0&1&0\\0&0&\bar1\end{pmatrix}$$

$$\mathtt{2C}=\begin{pmatrix}\bar1&0&0\\0&\bar1&0\\0&0&1\end{pmatrix}\quad \mathtt{2D}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar1\end{pmatrix}\quad \mathtt{2E}=\begin{pmatrix}0&\bar1&0\\\bar1&0&0\\0&0&\bar1\end{pmatrix}$$

$$\mathtt{2F}=\begin{pmatrix}1&\bar1&0\\0&\bar1&0\\0&0&\bar1\end{pmatrix}\quad \mathtt{2G}=\begin{pmatrix}1&0&0\\1&\bar1&0\\0&0&\bar1\end{pmatrix}\quad \mathtt{3Q}=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$$

$$\mathtt{3C}=\begin{pmatrix}0&\bar1&0\\1&\bar1&0\\0&0&1\end{pmatrix}\quad \mathtt{4C}=\begin{pmatrix}0&\bar1&0\\1&0&0\\0&0&1\end{pmatrix}\quad \mathtt{6C}=\begin{pmatrix}1&\bar1&0\\1&0&0\\0&0&1\end{pmatrix},$$

where only matrices of proper rotation are given (and required), since the corresponding matrices of improper rotation are created by the program for appropriate value of the r_i indicator. The first character of a symbol is the order of the axis of rotation and the second character specifies its orientation: in terms of direct-space lattice vectors, we have

$$\mathtt{A}=[100],\mathtt{B}=[010],\mathtt{C}=[001],\mathtt{D}=[110],$$
$$\mathtt{E}=[1\bar1 0],\mathtt{F}=[100],\mathtt{G}=[210]\ \text{and}\ \mathtt{Q}=[111]$$

for the standard orientations of the axes of rotation. Note that the axes `2F`, `2G`, `3C` and `6C` appear in trigonal and hexagonal space groups.

In the above scheme a space group is determined by one, two or at most three generators [see (A1.4.2.1)]. It should be pointed out that a convenient way of achieving a representation of the space group in any setting and relative to any origin is to start from the standard generators in Table A1.4.2.1 and let the computer program perform the appropriate transformation of the generators only, as in equations (1.4.4.4) and (1.4.4.5). The subsequent expansion of the transformed generators and the formation of the required products [see (A1.4.2.1) and (A1.4.2.2)] leads to the new representation of the space group.

In order to illustrate an explicit space-group symbol consider, for example, the symbol for the space group $Ia\bar3d$, as given in Table A1.4.2.1:

`ICC$I3Q000$P4C393$P2D933.`

The first three characters tell us that the Bravais lattice of this space group is of type `I`, that the space group is centrosymmetric and that it belongs to the cubic system. We then see that the generators are (i) an improper threefold axis along [111] (`I3Q`) with a zero translation part, (ii) a proper fourfold axis along [001] (`P4C`) with translation part (1/4, 3/4, 1/4) and (iii) a proper twofold axis along [110] (`P2D`) with translation part (3/4, 1/4, 1/4).

If we make use of the above-outlined interpretation of the explicit symbol (A1.4.2.3), the space-group symmetry transformations in direct space, corresponding to these three generators of the space group $Ia\bar3d$, become

Table A1.4.2.1. *Explicit symbols*

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
1	$P1$		`PAN$P1A000`
2	$P\bar{1}$		`PAC$I1A000`
3	$P2$	$P121$	`PMN$P2B000`
3	$P2$	$P112$	`PMN$P2C000`
4	$P2_1$	$P12_11$	`PMN$P2B060`
4	$P2_1$	$P112_1$	`PMN$P2C006`
5	$C2$	$C121$	`CMN$P2B000`
5	$C2$	$A121$	`AMN$P2B000`
5	$C2$	$I121$	`IMN$P2B000`
5	$C2$	$A112$	`AMN$P2C000`
5	$C2$	$B112$	`BMN$P2C000`
5	$C2$	$I112$	`IMN$P2C000`
6	Pm	$P1m1$	`PMN$I2B000`
6	Pm	$P11m$	`PMN$I2C000`
7	Pc	$P1c1$	`PMN$I2B006`
7	Pc	$P1n1$	`PMN$I2B606`
7	Pc	$P1a1$	`PMN$I2B600`
7	Pc	$P11a$	`PMN$I2C600`
7	Pc	$P11n$	`PMN$I2C660`
7	Pc	$P11b$	`PMN$I2C060`
8	Cm	$C1m1$	`CMN$I2B000`
8	Cm	$A1m1$	`AMN$I2B000`
8	Cm	$I1m1$	`IMN$I2B000`
8	Cm	$A11m$	`AMN$I2C000`
8	Cm	$B11m$	`BMN$I2C000`
8	Cm	$I11m$	`IMN$I2C000`
9	Cc	$C1c1$	`CMN$I2B006`
9	Cc	$A1n1$	`AMN$I2B606`
9	Cc	$I1a1$	`IMN$I2B600`
9	Cc	$A11a$	`AMN$I2C600`
9	Cc	$B11n$	`BMN$I2C660`
9	Cc	$I11b$	`IMN$I2C060`
10	$P2/m$	$P12/m1$	`PMC$I1A000$P2B000`
10	$P2/m$	$P112/m$	`PMC$I1A000$P2C000`
11	$P2_1/m$	$P12_1/m1$	`PMC$I1A000$P2B060`
11	$P2_1/m$	$P112_1/m$	`PMC$I1A000$P2C006`
12	$C2/m$	$C12/m1$	`CMC$I1A000$P2B000`
12	$C2/m$	$A12/m1$	`AMC$I1A000$P2B000`
12	$C2/m$	$I12/m1$	`IMC$I1A000$P2B000`
12	$C2/m$	$A112/m$	`AMC$I1A000$P2C000`
12	$C2/m$	$B112/m$	`BMC$I1A000$P2C000`
12	$C2/m$	$I112/m$	`IMC$I1A000$P2C000`
13	$P2/c$	$P12/c1$	`PMC$I1A000$P2B006`
13	$P2/c$	$P12/n1$	`PMC$I1A000$P2B606`
13	$P2/c$	$P12/a1$	`PMC$I1A000$P2B600`
13	$P2/c$	$P112/a$	`PMC$I1A000$P2C600`
13	$P2/c$	$P112/n$	`PMC$I1A000$P2C660`
13	$P2/c$	$P112/b$	`PMC$I1A000$P2C060`
14	$P2_1/c$	$P12_1/c1$	`PMC$I1A000$P2B066`
14	$P2_1/c$	$P12_1/n1$	`PMC$I1A000$P2B666`
14	$P2_1/c$	$P12_1/a1$	`PMC$I1A000$P2B660`
14	$P2_1/c$	$P112_1/a$	`PMC$I1A000$P2C606`
14	$P2_1/c$	$P112_1/n$	`PMC$I1A000$P2C666`
14	$P2_1/c$	$P112_1/b$	`PMC$I1A000$P2C066`
15	$C2/c$	$C12/c1$	`CMC$I1A000$P2B006`
15	$C2/c$	$A12/n1$	`AMC$I1A000$P2B606`
15	$C2/c$	$I12/a1$	`IMC$I1A000$P2B600`
15	$C2/c$	$A112/a$	`AMC$I1A000$P2C600`
15	$C2/c$	$B112/n$	`BMC$I1A000$P2C660`
15	$C2/c$	$I112/b$	`IMC$I1A000$P2C060`
16	$P222$		`PON$P2C000$P2A000`
17	$P222_1$		`PON$P2C006$P2A000`
18	$P2_12_12$		`PON$P2C000$P2A660`
19	$P2_12_12_1$		`PON$P2C606$P2A660`
20	$C222_1$		`CON$P2C006$P2A000`
21	$C222$		`CON$P2C000$P2A000`
22	$F222$		`FON$P2C000$P2A000`
23	$I222$		`ION$P2C000$P2A000`
24	$I2_12_12_1$		`ION$P2C606$P2A660`
25	$Pmm2$		`PON$P2C000$I2A000`
26	$Pmc2_1$		`PON$P2C006$I2A000`
27	$Pcc2$		`PON$P2C000$I2A006`
28	$Pma2$		`PON$P2C000$I2A600`
29	$Pca2_1$		`PON$P2C006$I2A606`
30	$Pnc2$		`PON$P2C000$I2A066`
31	$Pmn2_1$		`PON$P2C606$I2A000`
32	$Pba2$		`PON$P2C000$I2A660`
33	$Pna2_1$		`PON$P2C006$I2A666`
34	$Pnn2$		`PON$P2C000$I2A666`
35	$Cmm2$		`CON$P2C000$I2A000`
36	$Cmc2_1$		`CON$P2C006$I2A000`
37	$Ccc2$		`CON$P2C000$I2A006`
38	$Amm2$		`AON$P2C000$I2A000`
39	$Abm2$		`AON$P2C000$I2A060`
40	$Ama2$		`AON$P2C000$I2A600`
41	$Aba2$		`AON$P2C000$I2A660`
42	$Fmm2$		`FON$P2C000$I2A000`
43	$Fdd2$		`FON$P2C000$I2A333`
44	$Imm2$		`ION$P2C000$I2A000`
45	$Iba2$		`ION$P2C000$I2A660`
46	$Ima2$		`ION$P2C000$I2A600`
47	$Pmmm$		`POC$I1A000$P2C000$P2A000`
48	$Pnnn$	Origin 1	`POC$I1A666$P2C000$P2A000`
48	$Pnnn$	Origin 2	`POC$I1A000$P2C660$P2A066`
49	$Pccm$		`POC$I1A000$P2C000$P2A006`
50	$Pban$	Origin 1	`POC$I1A660$P2C000$P2A000`
50	$Pban$	Origin 2	`POC$I1A000$P2C660$P2A060`
51	$Pmma$		`POC$I1A000$P2C600$P2A600`
52	$Pnna$		`POC$I1A000$P2C600$P2A066`
53	$Pmna$		`POC$I1A000$P2C606$P2A000`
54	$Pcca$		`POC$I1A000$P2C600$P2A606`
55	$Pbam$		`POC$I1A000$P2C000$P2A660`
56	$Pccn$		`POC$I1A000$P2C660$P2A606`
57	$Pbcm$		`POC$I1A000$P2C006$P2A060`
58	$Pnnm$		`POC$I1A000$P2C000$P2A666`
59	$Pmmn$	Origin 1	`POC$I1A660$P2C000$P2A660`
59	$Pmmn$	Origin 2	`POC$I1A000$P2C660$P2A600`
60	$Pbcn$		`POC$I1A000$P2C666$P2A660`

Table A1.4.2.1. *Explicit symbols* (*cont.*)

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
61	$Pbca$		POC$I1A000$P2C606$P2A660
62	$Pnma$		POC$I1A000$P2C606$P2A666
63	$Cmcm$		COC$I1A000$P2C006$P2A000
64	$Cmca$		COC$I1A000$P2C066$P2A000
65	$Cmmm$		COC$I1A000$P2C000$P2A000
66	$Cccm$		COC$I1A000$P2C000$P2A006
67	$Cmma$		COC$I1A000$P2C060$P2A000
68	$Ccca$	Origin 1	COC$I1A066$P2C660$P2A660
68	$Ccca$	Origin 2	COC$I1A000$P2C600$P2A606
69	$Fmmm$		FOC$I1A000$P2C000$P2A000
70	$Fddd$	Origin 1	FOC$I1A333$P2C000$P2A000
70	$Fddd$	Origin 2	FOC$I1A000$P2C990$P2A099
71	$Immm$		IOC$I1A000$P2C000$P2A000
72	$Ibam$		IOC$I1A000$P2C000$P2A660
73	$Ibca$		IOC$I1A000$P2C606$P2A660
74	$Imma$		IOC$I1A000$P2C060$P2A000
75	$P4$		PTN$P4C000
76	$P4_1$		PTN$P4C003
77	$P4_2$		PTN$P4C006
78	$P4_3$		PTN$P4C009
79	$I4$		ITN$P4C000
80	$I4_1$		ITN$P4C063
81	$P\bar{4}$		PTN$I4C000
82	$I\bar{4}$		ITN$I4C000
83	$P4/m$		PTC$I1A000$P4C000
84	$P4_2/m$		PTC$I1A000$P4C006
85	$P4/n$	Origin 1	PTC$I1A660$P4C660
85	$P4/n$	Origin 2	PTC$I1A000$P4C600
86	$P4_2/n$	Origin 1	PTC$I1A666$P4C666
86	$P4_2/n$	Origin 2	PTC$I1A000$P4C066
87	$I4/m$		ITC$I1A000$P4C000
88	$I4_1/a$	Origin 1	ITC$I1A063$P4C063
88	$I4_1/a$	Origin 2	ITC$I1A000$P4C933
89	$P422$		PTN$P4C000$P2A000
90	$P42_12$		PTN$P4C660$P2A660
91	$P4_122$		PTN$P4C003$P2A006
92	$P4_12_12$		PTN$P4C663$P2A669
93	$P4_222$		PTN$P4C006$P2A000
94	$P4_22_12$		PTN$P4C666$P2A666
95	$P4_322$		PTN$P4C009$P2A006
96	$P4_32_12$		PTN$P4C669$P2A663
97	$I422$		ITN$P4C000$P2A000
98	$I4_122$		ITN$P4C063$P2A063
99	$P4mm$		PTN$P4C000$I2A000
100	$P4bm$		PTN$P4C000$I2A660
101	$P4_2cm$		PTN$P4C006$I2A006
102	$P4_2nm$		PTN$P4C666$I2A666
103	$P4cc$		PTN$P4C000$I2A006
104	$P4nc$		PTN$P4C000$I2A666
105	$P4_2mc$		PTN$P4C006$I2A000
106	$P4_2bc$		PTN$P4C006$I2A660
107	$I4mm$		ITN$P4C000$I2A000
108	$I4cm$		ITN$P4C000$I2A006
109	$I4_1md$		ITN$P4C063$I2A666
110	$I4_1cd$		ITN$P4C063$I2A660
111	$P\bar{4}2m$		PTN$I4C000$P2A000
112	$P\bar{4}2c$		PTN$I4C000$P2A006
113	$P\bar{4}2_1m$		PTN$I4C000$P2A660
114	$P\bar{4}2_1c$		PTN$I4C000$P2A666
115	$P\bar{4}m2$		PTN$I4C000$P2D000
116	$P\bar{4}c2$		PTN$I4C000$P2D006
117	$P\bar{4}b2$		PTN$I4C000$P2D660
118	$P\bar{4}n2$		PTN$I4C000$P2D666
119	$I\bar{4}m2$		ITN$I4C000$P2D000
120	$I\bar{4}c2$		ITN$I4C000$P2D006
121	$I\bar{4}2m$		ITN$I4C000$P2A000
122	$I\bar{4}2d$		ITN$I4C000$P2A609
123	$P4/mmm$		PTC$I1A000$P4C000$P2A000
124	$P4/mcc$		PTC$I1A000$P4C000$P2A006
125	$P4/nbm$	Origin 1	PTC$I1A660$P4C000$P2A000
125	$P4/nbm$	Origin 2	PTC$I1A000$P4C600$P2A060
126	$P4/nnc$	Origin 1	PTC$I1A666$P4C000$P2A000
126	$P4/nnc$	Origin 2	PTC$I1A000$P4C600$P2A066
127	$P4/mbm$		PTC$I1A000$P4C000$P2A660
128	$P4/mnc$		PTC$I1A000$P4C000$P2A666
129	$P4/nmm$	Origin 1	PTC$I1A660$P4C660$P2A660
129	$P4/nmm$	Origin 2	PTC$I1A000$P4C600$P2A600
130	$P4/ncc$	Origin 1	PTC$I1A660$P4C660$P2A666
130	$P4/ncc$	Origin 2	PTC$I1A000$P4C600$P2A606
131	$P4_2/mmc$		PTC$I1A000$P4C006$P2A000
132	$P4_2/mcm$		PTC$I1A000$P4C006$P2A006
133	$P4_2/nbc$	Origin 1	PTC$I1A666$P4C666$P2A006
133	$P4_2/nbc$	Origin 2	PTC$I1A000$P4C606$P2A060
134	$P4_2/nnm$	Origin 1	PTC$I1A666$P4C666$P2A000
134	$P4_2/nnm$	Origin 2	PTC$I1A000$P4C606$P2A066
135	$P4_2/mbc$		PTC$I1A000$P4C006$P2A660
136	$P4_2/mnm$		PTC$I1A000$P4C666$P2A666
137	$P4_2/nmc$	Origin 1	PTC$I1A666$P4C666$P2A666
137	$P4_2/nmc$	Origin 2	PTC$I1A000$P4C606$P2A600
138	$P4_2/ncm$	Origin 1	PTC$I1A666$P4C666$P2A660
138	$P4_2/ncm$	Origin 2	PTC$I1A000$P4C606$P2A606
139	$I4/mmm$		ITC$I1A000$P4C000$P2A000
140	$I4/mcm$		ITC$I1A000$P4C000$P2A006
141	$I4_1/amd$	Origin 1	ITC$I1A063$P4C063$P2A063
141	$I4_1/amd$	Origin 2	ITC$I1A000$P4C393$P2A000
142	$I4_1/acd$	Origin 1	ITC$I1A063$P4C063$P2A069
142	$I4_1/acd$	Origin 2	ITC$I1A000$P4C393$P2A006
143	$P3$		PRN$P3C000
144	$P3_1$		PRN$P3C004
145	$P3_2$		PRN$P3C008
146	$R3$	Hexagonal axes	RRN$P3C000
146	$R3$	Rhombohedral axes	PRN$P3Q000
147	$P\bar{3}$		PRC$I3C000
148	$R\bar{3}$	Hexagonal axes	RRC$I3C000
148	$R\bar{3}$	Rhombohedral axes	PRC$I3Q000
149	$P312$		PRN$P3C000$P2G000
150	$P321$		PRN$P3C000$P2F000
151	$P3_112$		PRN$P3C004$P2G000

Table A1.4.2.1. *Explicit symbols* (*cont.*)

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
152	$P3_121$		`PRN$P3C004$P2F008`
153	$P3_212$		`PRN$P3C008$P2G000`
154	$P3_221$		`PRN$P3C008$P2F004`
155	$R32$	Hexagonal axes	`RRN$P3C000$P2F000`
155	$R32$	Rhombohedral axes	`PRN$P3Q000$P2E000`
156	$P3m1$		`PRN$P3C000$I2F000`
157	$P31m$		`PRN$P3C000$I2G000`
158	$P3c1$		`PRN$P3C000$I2F006`
159	$P31c$		`PRN$P3C000$I2G006`
160	$R3m$	Hexagonal axes	`RRN$P3C000$I2F000`
160	$R3m$	Rhombohedral axes	`PRN$P3Q000$I2E000`
161	$R3c$	Hexagonal axes	`RRN$P3C000$I2F006`
161	$R3c$	Rhombohedral axes	`PRN$P3Q000$I2E666`
162	$P\bar{3}1m$		`PRC$I3C000$P2G000`
163	$P\bar{3}1c$		`PRC$I3C000$P2G006`
164	$P\bar{3}m1$		`PRC$I3C000$P2F000`
165	$P\bar{3}c1$		`PRC$I3C000$P2F006`
166	$R\bar{3}m$	Hexagonal axes	`RRC$I3C000$P2F000`
166	$R\bar{3}m$	Rhombohedral axes	`PRC$I3Q000$P2E000`
167	$R\bar{3}c$	Hexagonal axes	`RRC$I3C000$P2F006`
167	$R\bar{3}c$	Rhombohedral axes	`PRC$I3Q000$P2E666`
168	$P6$		`PHN$P6C000`
169	$P6_1$		`PHN$P6C002`
170	$P6_5$		`PHN$P6C005`
171	$P6_2$		`PHN$P6C004`
172	$P6_4$		`PHN$P6C008`
173	$P6_3$		`PHN$P6C006`
174	$P\bar{6}$		`PHN$I6C000`
175	$P6/m$		`PHC$I1A000$P6C000`
176	$P6_3/m$		`PHC$I1A000$P6C006`
177	$P622$		`PHN$P6C000$P2F000`
178	$P6_122$		`PHN$P6C002$P2F000`
179	$P6_522$		`PHN$P6C005$P2F000`
180	$P6_222$		`PHN$P6C004$P2F000`
181	$P6_422$		`PHN$P6C008$P2F000`
182	$P6_322$		`PHN$P6C006$P2F000`
183	$P6mm$		`PHN$P6C000$I2F000`
184	$P6cc$		`PHN$P6C000$I2F006`
185	$P6_3cm$		`PHN$P6C006$I2F006`
186	$P6_3mc$		`PHN$P6C006$I2F000`
187	$P\bar{6}m2$		`PHN$I6C000$P2G000`
188	$P\bar{6}c2$		`PHN$I6C006$P2G000`
189	$P\bar{6}2m$		`PHN$I6C000$P2F000`
190	$P\bar{6}2c$		`PHN$I6C006$P2F000`
191	$P6/mmm$		`PHC$I1A000$P6C000$P2F000`

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
192	$P6/mcc$		`PHC$I1A000$P6C000$P2F006`
193	$P6_3/mcm$		`PHC$I1A000$P6C006$P2F006`
194	$P6_3/mmc$		`PHC$I1A000$P6C006$P2F000`
195	$P23$		`PCN$P3Q000$P2C000$P2A000`
196	$F23$		`FCN$P3Q000$P2C000$P2A000`
197	$I23$		`ICN$P3Q000$P2C000$P2A000`
198	$P2_13$		`PCN$P3Q000$P2C606$P2A660`
199	$I2_13$		`ICN$P3Q000$P2C606$P2A660`
200	$Pm\bar{3}$		`PCC$I3Q000$P2C000$P2A000`
201	$Pn\bar{3}$	Origin 1	`PCC$I3Q666$P2C000$P2A000`
201	$Pn\bar{3}$	Origin 2	`PCC$I3Q000$P2C660$P2A066`
202	$Fm\bar{3}$		`FCC$I3Q000$P2C000$P2A000`
203	$Fd\bar{3}$	Origin 1	`FCC$I3Q333$P2C000$P2A000`
203	$Fd\bar{3}$	Origin 2	`FCC$I3Q000$P2C330$P2A033`
204	$Im\bar{3}$		`ICC$I3Q000$P2C000$P2A000`
205	$Pa\bar{3}$		`PCC$I3Q000$P2C606$P2A660`
206	$Ia\bar{3}$		`ICC$I3Q000$P2C606$P2A660`
207	$P432$		`PCN$P3Q000$P4C000$P2D000`
208	$P4_232$		`PCN$P3Q000$P4C666$P2D666`
209	$F432$		`FCN$P3Q000$P4C000$P2D000`
210	$F4_132$		`FCN$P3Q000$P4C993$P2D939`
211	$I432$		`ICN$P3Q000$P4C000$P2D000`
212	$P4_332$		`PCN$P3Q000$P4C939$P2D399`
213	$P4_132$		`PCN$P3Q000$P4C393$P2D933`
214	$I4_132$		`ICN$P3Q000$P4C393$P2D933`
215	$P\bar{4}3m$		`PCN$P3Q000$I4C000$I2D000`
216	$F\bar{4}3m$		`FCN$P3Q000$I4C000$I2D000`
217	$I\bar{4}3m$		`ICN$P3Q000$I4C000$I2D000`
218	$P\bar{4}3n$		`PCN$P3Q000$I4C666$I2D666`
219	$F\bar{4}3c$		`FCN$P3Q000$I4C666$I2D666`
220	$I\bar{4}3d$		`ICN$P3Q000$I4C939$I2D399`
221	$Pm\bar{3}m$		`PCC$I3Q000$P4C000$P2D000`
222	$Pn\bar{3}n$	Origin 1	`PCC$I3Q666$P4C000$P2D000`
222	$Pn\bar{3}n$	Origin 2	`PCC$I3Q000$P4C600$P2D006`
223	$Pm\bar{3}n$		`PCC$I3Q000$P4C666$P2D666`
224	$Pn\bar{3}m$	Origin 1	`PCC$I3Q666$P4C666$P2D666`
224	$Pn\bar{3}m$	Origin 2	`PCC$I3Q000$P4C066$P2D660`
225	$Fm\bar{3}m$		`FCC$I3Q000$P4C000$P2D000`
226	$Fm\bar{3}c$		`FCC$I3Q000$P4C666$P2D666`
227	$Fd\bar{3}m$	Origin 1	`FCC$I3Q333$P4C993$P2D939`
227	$Fd\bar{3}m$	Origin 2	`FCC$I3Q000$P4C693$P2D936`
228	$Fd\bar{3}c$	Origin 1	`FCC$I3Q999$P4C993$P2D939`
228	$Fd\bar{3}c$	Origin 2	`FCC$I3Q000$P4C093$P2D930`
229	$Im\bar{3}m$		`ICC$I3Q000$P4C000$P2D000`
230	$Ia\bar{3}d$		`ICC$I3Q000$P4C393$P2D933`

Table A1.4.2.2. *Lattice symbol L*

The lattice symbol L implies Seitz matrices for the lattice translations. For noncentrosymmetric lattices the rotation parts of the Seitz matrices are for *1* (see Table A1.4.2.4). For centrosymmetric lattices the rotation parts are *1* and *−1*. The translation parts in the fourth columns of the Seitz matrices are listed in the last column of the table. The total number of matrices implied by each symbol is given by **nS**.

Noncentrosymmetric		Centrosymmetric		
Symbol	**nS**	Symbol	**nS**	Implied lattice translation(s)
P	1	−P	2	0, 0, 0
A	2	−A	4	0, 0, 0 $0, \frac{1}{2}, \frac{1}{2}$
B	2	−B	4	0, 0, 0 $\frac{1}{2}, 0, \frac{1}{2}$
C	2	−C	4	0, 0, 0 $\frac{1}{2}, \frac{1}{2}, 0$
I	2	−I	4	0, 0, 0 $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
R	3	−R	6	0, 0, 0 $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$
H	3	−H	6	0, 0, 0 $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
F	4	−F	8	0, 0, 0 $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$

$$\left[\begin{pmatrix}0&0&\bar{1}\\ \bar{1}&0&0\\ 0&\bar{1}&0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix}+\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}\right]=\begin{pmatrix}\bar{z}\\ \bar{x}\\ \bar{y}\end{pmatrix},$$

$$\left[\begin{pmatrix}0&\bar{1}&0\\ 1&0&0\\ 0&0&1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix}+\begin{pmatrix}\frac{1}{4}\\ \frac{3}{4}\\ \frac{1}{4}\end{pmatrix}\right]=\begin{pmatrix}\frac{1}{4}-y\\ \frac{3}{4}+x\\ \frac{1}{4}+z\end{pmatrix},$$

$$\left[\begin{pmatrix}0&1&0\\ 1&0&0\\ 0&0&\bar{1}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix}+\begin{pmatrix}\frac{3}{4}\\ \frac{1}{4}\\ \frac{1}{4}\end{pmatrix}\right]=\begin{pmatrix}\frac{3}{4}+y\\ \frac{1}{4}+x\\ \frac{1}{4}-z\end{pmatrix}.$$

The corresponding symmetry transformations in reciprocal space, in the notation of Section 1.4.4, are

$$\left[(hkl)\begin{pmatrix}0&0&\bar{1}\\ \bar{1}&0&0\\ 0&\bar{1}&0\end{pmatrix}:-(hkl)\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}\right]=[\overline{klh}:0];$$

similarly, $[k\bar{h}l:-131/4]$ and $[kh\bar{l}:-311/4]$ are obtained from the second and third generator of $Ia\bar{3}d$, respectively.

The first column of Table A1.4.2.1 lists the conventional space-group number. The second column shows the conventional short Hermann–Mauguin or international space-group symbol, and the third column, *Comments*, shows the full international space-group symbol *only* for the different settings of the monoclinic space groups that are given in the main space-group tables of *IT* A (1983). Other comments pertain to the choice of the space-group origin – where there are alternatives – and to axial systems. The fourth column shows the explicit space-group symbols described above for each of the settings considered in *IT* A (1983).

A1.4.2.3. *Hall symbols* (S. R. Hall and R. W. Grosse-Kunstleve)

The explicit-origin space-group notation proposed by Hall (1981*a*) is based on a subset of the symmetry operations, in the form of Seitz matrices, sufficient to uniquely define a space group. The concise unambiguous nature of this notation makes it well suited to handling symmetry in computing and database applications.

Table A1.4.2.7 lists space-group notation in several formats. The first column of Table A1.4.2.7 lists the space-group numbers with axis codes appended to identify the non-standard settings. The second column lists the Hermann–Mauguin symbols in computer-entry format with appended codes to identify the origin and cell choice when there are alternatives. The general forms of the Hall notation are listed in the fourth column and the computer-entry representations of these symbols are listed in the third column. The computer-entry format is the general notation expressed as case-insensitive ASCII characters with the overline (bar) symbol replaced by a minus sign.

The Hall notation has the general form:

$$\mathbf{L}[\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}]_{\mathbf{1}}\ldots[\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}]_{\mathbf{p}}\mathbf{V}. \tag{A1.4.2.4}$$

L is the symbol specifying the lattice translational symmetry (see Table A1.4.2.2). The integral translations are implicitly included in the set of generators. If **L** has a leading minus sign, it also specifies an inversion centre at the origin. $[\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}]_{\mathbf{n}}$ specifies the 4 × 4 Seitz matrix $\mathbf{S}_{\mathbf{n}}$ of a symmetry element in the minimum set which defines the space-group symmetry (see Tables A1.4.2.3 to A1.4.2.6), and **p** is the number of elements in the set. **V** is a change-of-basis operator needed for less common descriptions of the space-group symmetry.

Table A1.4.2.3. *Translation symbol T*

The symbol T specifies the translation elements of a Seitz matrix. Alphabetical symbols (given in the first column) specify translations along a fixed direction. Numerical symbols (given in the third column) specify translations as a fraction of the rotation order |N| and in the direction of the implied or explicitly defined axis.

Translation symbol	Translation vector	Subscript symbol	Fractional translation
a	$\frac{1}{2}, 0, 0$	*1* in 3_1	$\frac{1}{3}$
b	$0, \frac{1}{2}, 0$	*2* in 3_2	$\frac{2}{3}$
c	$0, 0, \frac{1}{2}$	*1* in 4_1	$\frac{1}{4}$
n	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	*3* in 4_3	$\frac{3}{4}$
u	$\frac{1}{4}, 0, 0$	*1* in 6_1	$\frac{1}{6}$
v	$0, \frac{1}{4}, 0$	*2* in 6_2	$\frac{1}{3}$
w	$0, 0, \frac{1}{4}$	*4* in 6_4	$\frac{2}{3}$
d	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	*5* in 6_5	$\frac{5}{6}$

Table A1.4.2.4. *Rotation matrices for principal axes*

The 3 × 3 matrices for *proper* rotations along the three principal unit-cell directions are given below. The matrices for *improper* rotations (−*1*, −*2*, −*3*, −*4* and −*6*) are identical except that the signs of the elements are reversed.

Axis	Symbol A	Rotation order *1*	*2*	*3*	*4*	*6*
a	*x*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&\bar{1}\\0&1&0\end{pmatrix}$
b	*y*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&1\end{pmatrix}$
c	*z*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$

The matrix symbol $\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}$ is composed of three parts: **N** is the symbol denoting the |N|-fold order of the rotation matrix (see Tables A1.4.2.4, A1.4.2.5 and A1.4.2.6), **T** is a subscript symbol denoting the *translation* vector (see Table A1.4.2.3) and **A** is a superscript symbol denoting the *axis* of rotation.

The computer-entry format of the Hall notation contains the rotation-order symbol **N** as positive integers *1*, *2*, *3*, *4*, or *6* for proper rotations and as negative integers −*1*, −*2*, −*3*, −*4* or −*6* for improper rotations. The **T** translation symbols *1*, *2*, *3*, *4*, *5*, *6*, *a*, *b*, *c*, *n*, *u*, *v*, *w*, *d* are described in Table A1.4.2.3. These translations apply additively [*e.g.* *ad* signifies a $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$ translation]. The **A** axis symbols *x*, *y*, *z* denote rotations about the axes **a**, **b** and **c**, respectively (see Table A1.4.2.4). The axis symbols ″ and ′ signal rotations about the body-diagonal vectors **a** + **b** (or alternatively **b** + **c** or **c** + **a**) and **a** − **b** (or alternatively **b** − **c** or **c** − **a**) (see Table A1.4.2.5). The axis symbol * always refers to a threefold rotation along **a** + **b** + **c** (see Table A1.4.2.6).

Table A1.4.2.5. *Rotation matrices for face-diagonal axes*

The symbols for face-diagonal twofold rotations are *2*′ and *2*″. The face-diagonal axis direction is determined by the axis of the preceding rotation N^x, N^y or N^z. Note that the single prime ′ is the default and may be omitted.

Preceding rotation	Rotation	Axis	Matrix
N^x	*2*′	**b** − **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{pmatrix}$
	2″	**b** + **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{pmatrix}$
N^y	*2*′	**a** − **c**	$\begin{pmatrix}0&0&\bar{1}\\0&\bar{1}&0\\\bar{1}&0&0\end{pmatrix}$
	2″	**a** + **c**	$\begin{pmatrix}0&0&1\\0&\bar{1}&0\\1&0&0\end{pmatrix}$
N^z	*2*′	**a** − **b**	$\begin{pmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{pmatrix}$
	2″	**a** + **b**	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$

The change-of-basis operator **V** has the general form (v_x, v_y, v_z). The vectors v_x, v_y and v_z are specified by

$$v_x = r_{1,1}X + r_{1,2}Y + r_{1,3}Z + \mathbf{t}_1$$
$$v_y = r_{2,1}X + r_{2,2}Y + r_{2,3}Z + \mathbf{t}_2\,,$$
$$v_z = r_{3,1}X + r_{3,2}Y + r_{3,3}Z + \mathbf{t}_3$$

where $r_{i,j}$ and $\mathbf{t}_i$ are fractions or real numbers. Terms in which $r_{i,j}$ or $\mathbf{t}_i$ are zero need not be specified. The 4 × 4 change-of-basis matrix operator **V** is defined as

$$\mathbf{V} = \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & \mathbf{t}_1 \\ r_{2,1} & r_{2,2} & r_{2,3} & \mathbf{t}_2 \\ r_{3,1} & r_{3,2} & r_{3,3} & \mathbf{t}_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The transformed symmetry operations are derived from the specified Seitz matrices $\mathbf{S_n}$ as

$$\mathbf{S}'_{\mathbf{n}} = \mathbf{V} \cdot \mathbf{S_n} \cdot \mathbf{V}^{-1}$$

and from the integral translations $\mathbf{t}(1, 0, 0)$, $\mathbf{t}(0, 1, 0)$ and $\mathbf{t}(0, 0, 1)$ as

$$(\mathbf{t}'_{\mathbf{n}}, \mathbf{1})^T = \mathbf{V} \cdot (\mathbf{t_n}, \mathbf{1})^T.$$

A shorthand form of **V** may be used when the change-of-basis operator only translates the origin of the basis system. In this form v_x, v_y and v_z are specified simply as shifts in twelfths, implying the matrix operator

Table A1.4.2.6. *Rotation matrix for the body-diagonal axis*

The symbol for the threefold rotation in the **a** + **b** + **c** direction is *3**. Note that for cubic space groups the body-diagonal axis is implied and the asterisk * may be omitted.

Axis	Rotation	Matrix
a + **b** + **c**	*3**	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$

$$\mathbf{V} = \begin{pmatrix} 1 & 0 & 0 & v_x/12 \\ 0 & 1 & 0 & v_y/12 \\ 0 & 0 & 1 & v_z/12 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In the shorthand form of **V**, the commas separating the vectors may be omitted.

A1.4.2.3.1. *Default axes*

For most symbols the rotation axes applicable to each **N** are implied and an explicit axis symbol **A** is not needed. The rules for *default* axis directions are:

(i) the *first* rotation or roto-inversion has an axis direction of **c**;

(ii) the *second* rotation (if |N| is 2) has an axis direction of **a** if preceded by an |N| of 2 or 4, **a**−**b** if preceded by an |N| of 3 or 6;

(iii) the *third* rotation (if |N| is 3) has an axis direction of **a** + **b** + **c**.

A1.4.2.3.2. *Example matrices*

The following examples show how the notation expands to Seitz matrices.

The notation $\bar{2}_c^x$ represents an improper twofold rotation along **a** and a **c**/2 translation:

$$-2\mathrm{xc} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation *3** represents a threefold rotation along **a** + **b** + **c**:

$$3^* = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 4_{vw} represents a fourfold rotation along **c** (implied) and translation of **b**/4 and **c**/4:

$$4\mathrm{vw} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 6_1 2 (0 0 −1) represents a 6_1 screw along **c**, a twofold rotation along **a** − **b** and an origin shift of −**c**/12. Note that the 6_1 matrix is unchanged by the shifted origin whereas the *2* matrix is changed by −**c**/6.

$$61\ 2\ (0\ 0\ -1) = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \frac{5}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The change-of-basis vector (0 0 −1) could also be entered as (*x*, *y*, *z* − 1/12).

The *reverse setting of the R-centred lattice* (hexagonal axes) is specified using a change-of-basis transformation applied to the standard *obverse setting* (see Table A1.4.2.2). The obverse Seitz matrices are

$$\mathrm{R}\ 3 = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The reverse-setting Seitz matrices are

$$\mathrm{R}\ 3\ (-\mathrm{x}, -\mathrm{y}, \mathrm{z}) = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The conventional primitive hexagonal lattice may be transformed to a *C-centred orthohexagonal setting* using the change-of-basis operator

$$\mathrm{P}\ 6\ (\mathrm{x} - 1/2\mathrm{y}, 1/2\mathrm{y}, \mathrm{z}) = \begin{pmatrix} \frac{1}{2} & -\frac{3}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In this case the lattice translation for the *C* centring is obtained by transforming the integral translation **t**(0, 1, 0):

$$\boldsymbol{V} \cdot (0\quad 1\quad 0\quad 1)^T = \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \left(-\tfrac{1}{2}\quad \tfrac{1}{2}\quad 0\quad 1\right)^T.$$

The standard setting of an *I*-centred tetragonal space group may be transformed to a primitive setting using the change-of-basis operator

$$\mathrm{I}\ 4\ (\mathrm{y} + \mathrm{z}, \mathrm{x} + \mathrm{z}, \mathrm{x} + \mathrm{y}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Note that in the primitive setting, the fourfold axis is along **a** + **b**.

Table A1.4.2.7. *Hall symbols*

The first column, n:c, lists the space-group numbers and axis codes separated by a colon. The second column lists the Hermann–Mauguin symbols in computer-entry format. The third column lists the Hall symbols in computer-entry format and the fourth column lists the Hall symbols as described in Tables A1.4.2.2–A1.4.2.6.

n:c	H–M entry	Hall entry	Hall symbol
1	P 1	p 1	$P\ 1$
2	P -1	-p 1	$\bar{P}\ 1$
3:b	P 1 2 1	p 2y	$P\ 2^{y}$
3:c	P 1 1 2	p 2	$P\ 2$
3:a	P 2 1 1	p 2x	$P\ 2^{x}$
4:b	P 1 21 1	p 2yb	$P\ 2^{y}_{b}$
4:c	P 1 1 21	p 2c	$P\ 2_{c}$
4:a	P 21 1 1	p 2xa	$P\ 2^{x}_{a}$
5:b1	C 1 2 1	c 2y	$C\ 2^{y}$
5:b2	A 1 2 1	a 2y	$A\ 2^{y}$
5:b3	I 1 2 1	i 2y	$I\ 2^{y}$
5:c1	A 1 1 2	a 2	$A\ 2$
5:c2	B 1 1 2	b 2	$B\ 2$
5:c3	I 1 1 2	i 2	$I\ 2$
5:a1	B 2 1 1	b 2x	$B\ 2^{x}$
5:a2	C 2 1 1	c 2x	$C\ 2^{x}$
5:a3	I 2 1 1	i 2x	$I\ 2^{x}$
6:b	P 1 m 1	p -2y	$P\ \bar{2}^{y}$
6:c	P 1 1 m	p -2	$P\ \bar{2}$
6:a	P m 1 1	p -2x	$P\ \bar{2}^{x}$
7:b1	P 1 c 1	p -2yc	$P\ \bar{2}^{y}_{c}$
7:b2	P 1 n 1	p -2yac	$P\ \bar{2}^{y}_{ac}$
7:b3	P 1 a 1	p -2ya	$P\ \bar{2}^{y}_{a}$
7:c1	P 1 1 a	p -2a	$P\ \bar{2}_{a}$
7:c2	P 1 1 n	p -2ab	$P\ \bar{2}_{ab}$
7:c3	P 1 1 b	p -2b	$P\ \bar{2}_{b}$
7:a1	P b 1 1	p -2xb	$P\ \bar{2}^{x}_{b}$
7:a2	P n 1 1	p -2xbc	$P\ \bar{2}^{x}_{bc}$
7:a3	P c 1 1	p -2xc	$P\ \bar{2}^{x}_{c}$
8:b1	C 1 m 1	c -2y	$C\ \bar{2}^{y}$
8:b2	A 1 m 1	a -2y	$A\ \bar{2}^{y}$
8:b3	I 1 m 1	i -2y	$I\ \bar{2}^{y}$
8:c1	A 1 1 m	a -2	$A\ \bar{2}$
8:c2	B 1 1 m	b -2	$B\ \bar{2}$
8:c3	I 1 1 m	i -2	$I\ \bar{2}$
8:a1	B m 1 1	b -2x	$B\ \bar{2}^{x}$
8:a2	C m 1 1	c -2x	$C\ \bar{2}^{x}$
8:a3	I m 1 1	i -2x	$I\ \bar{2}^{x}$
9:b1	C 1 c 1	c -2yc	$C\ \bar{2}^{y}_{c}$
9:b2	A 1 n 1	a -2yab	$A\ \bar{2}^{y}_{ab}$
9:b3	I 1 a 1	i -2ya	$I\ \bar{2}^{y}_{a}$
9:-b1	A 1 a 1	a -2ya	$A\ \bar{2}^{y}_{a}$
9:-b2	C 1 n 1	c -2yac	$C\ \bar{2}^{y}_{ac}$
9:-b3	I 1 c 1	i -2yc	$I\ \bar{2}^{y}_{c}$
9:c1	A 1 1 a	a -2a	$A\ \bar{2}_{a}$
9:c2	B 1 1 n	b -2ab	$B\ \bar{2}_{ab}$
9:c3	I 1 1 b	i -2b	$I\ \bar{2}_{b}$
9:-c1	B 1 1 b	b -2b	$B\ \bar{2}_{b}$
9:-c2	A 1 1 n	a -2ab	$A\ \bar{2}_{ab}$
9:-c3	I 1 1 a	i -2a	$I\ \bar{2}_{a}$
9:a1	B b 1 1	b -2xb	$B\ \bar{2}^{x}_{b}$
9:a2	C n 1 1	c -2xac	$C\ \bar{2}^{x}_{ac}$
9:a3	I c 1 1	i -2xc	$I\ \bar{2}^{x}_{c}$
9:-a1	C c 1 1	c -2xc	$C\ \bar{2}^{x}_{c}$
9:-a2	B n 1 1	b -2xab	$B\ \bar{2}^{x}_{ab}$
9:-a3	I b 1 1	i -2xb	$I\ \bar{2}^{x}_{b}$
10:b	P 1 2/m 1	-p 2y	$\bar{P}\ 2^{y}$
10:c	P 1 1 2/m	-p 2	$\bar{P}\ 2$
10:a	P 2/m 1 1	-p 2x	$\bar{P}\ 2^{x}$
11:b	P 1 21/m 1	-p 2yb	$\bar{P}\ 2^{y}_{b}$
11:c	P 1 1 21/m	-p 2c	$\bar{P}\ 2_{c}$
11:a	P 21/m 1 1	-p 2xa	$\bar{P}\ 2^{x}_{a}$
12:b1	C 1 2/m 1	-c 2y	$\bar{C}\ 2^{y}$
12:b2	A 1 2/m 1	-a 2y	$\bar{A}\ 2^{y}$
12:b3	I 1 2/m 1	-i 2y	$\bar{I}\ 2^{y}$
12:c1	A 1 1 2/m	-a 2	$\bar{A}\ 2$
12:c2	B 1 1 2/m	-b 2	$\bar{B}\ 2$
12:c3	I 1 1 2/m	-i 2	$\bar{I}\ 2$
12:a1	B 2/m 1 1	-b 2x	$\bar{B}\ 2^{x}$
12:a2	C 2/m 1 1	-c 2x	$\bar{C}\ 2^{x}$
12:a3	I 2/m 1 1	-i 2x	$\bar{I}\ 2^{x}$
13:b1	P 1 2/c 1	-p 2yc	$\bar{P}\ 2^{y}_{c}$
13:b2	P 1 2/n 1	-p 2yac	$\bar{P}\ 2^{y}_{ac}$
13:b3	P 1 2/a 1	-p 2ya	$\bar{P}\ 2^{y}_{a}$
13:c1	P 1 1 2/a	-p 2a	$\bar{P}\ 2_{a}$
13:c2	P 1 1 2/n	-p 2ab	$\bar{P}\ 2_{ab}$
13:c3	P 1 1 2/b	-p 2b	$\bar{P}\ 2_{b}$
13:a1	P 2/b 1 1	-p 2xb	$\bar{P}\ 2^{x}_{b}$
13:a2	P 2/n 1 1	-p 2xbc	$\bar{P}\ 2^{x}_{bc}$
13:a3	P 2/c 1 1	-p 2xc	$\bar{P}\ 2^{x}_{c}$
14:b1	P 1 21/c 1	-p 2ybc	$\bar{P}\ 2^{y}_{bc}$
14:b2	P 1 21/n 1	-p 2yn	$\bar{P}\ 2^{y}_{n}$
14:b3	P 1 21/a 1	-p 2yab	$\bar{P}\ 2^{y}_{ab}$
14:c1	P 1 1 21/a	-p 2ac	$\bar{P}\ 2_{ac}$
14:c2	P 1 1 21/n	-p 2n	$\bar{P}\ 2_{n}$
14:c3	P 1 1 21/b	-p 2bc	$\bar{P}\ 2_{bc}$
14:a1	P 21/b 1 1	-p 2xab	$\bar{P}\ 2^{x}_{ab}$
14:a2	P 21/n 1 1	-p 2xn	$\bar{P}\ 2^{x}_{n}$
14:a3	P 21/c 1 1	-p 2xac	$\bar{P}\ 2^{x}_{ac}$
15:b1	C 1 2/c 1	-c 2yc	$\bar{C}\ 2^{y}_{c}$
15:b2	A 1 2/n 1	-a 2yab	$\bar{A}\ 2^{y}_{ab}$
15:b3	I 1 2/a 1	-i 2ya	$\bar{I}\ 2^{y}_{a}$
15:-b1	A 1 2/a 1	-a 2ya	$\bar{A}\ 2^{y}_{a}$
15:-b2	C 1 2/n 1	-c 2yac	$\bar{C}\ 2^{y}_{ac}$
15:-b3	I 1 2/c 1	-i 2yc	$\bar{I}\ 2^{y}_{c}$
15:c1	A 1 1 2/a	-a 2a	$\bar{A}\ 2_{a}$
15:c2	B 1 1 2/n	-b 2ab	$\bar{B}\ 2_{ab}$
15:c3	I 1 1 2/b	-i 2b	$\bar{I}\ 2_{b}$
15:-c1	B 1 1 2/b	-b 2b	$\bar{B}\ 2_{b}$
15:-c2	A 1 1 2/n	-a 2ab	$\bar{A}\ 2_{ab}$
15:-c3	I 1 1 2/a	-i 2a	$\bar{I}\ 2_{a}$
15:a1	B 2/b 1 1	-b 2xb	$\bar{B}\ 2^{x}_{b}$
15:a2	C 2/n 1 1	-c 2xac	$\bar{C}\ 2^{x}_{ac}$
15:a3	I 2/c 1 1	-i 2xc	$\bar{I}\ 2^{x}_{c}$
15:-a1	C 2/c 1 1	-c 2xc	$\bar{C}\ 2^{x}_{c}$
15:-a2	B 2/n 1 1	-b 2xab	$\bar{B}\ 2^{x}_{ab}$
15:-a3	I 2/b 1 1	-i 2xb	$\bar{I}\ 2^{x}_{b}$
16	P 2 2 2	p 2 2	$P\ 2\ 2$

Table A1.4.2.7. *Hall symbols* (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
17	P 2 2 21	p 2c 2	P 2_c 2
17:cab	P 21 2 2	p 2a 2a	P 2_a 2_a
17:bca	P 2 21 2	p 2 2b	P 2 2_b
18	P 21 21 2	p 2 2ab	P 2 2_{ab}
18:cab	P 2 21 21	p 2bc 2	P 2_{bc} 2
18:bca	P 21 2 21	p 2ac 2ac	P 2_{ac} 2_{ac}
19	P 21 21 21	p 2ac 2ab	P 2_{ac} 2_{ab}
20	C 2 2 21	c 2c 2	C 2_c 2
20:cab	A 21 2 2	a 2a 2a	A 2_a 2_a
20:bca	B 2 21 2	b 2 2b	B 2 2_b
21	C 2 2 2	c 2 2	C 2 2
21:cab	A 2 2 2	a 2 2	A 2 2
21:bca	B 2 2 2	b 2 2	B 2 2
22	F 2 2 2	f 2 2	F 2 2
23	I 2 2 2	i 2 2	I 2 2
24	I 21 21 21	i 2b 2c	I 2_b 2_c
25	P m m 2	p 2 -2	P 2 $\bar{2}$
25:cab	P 2 m m	p -2 2	P $\bar{2}$ 2
25:bca	P m 2 m	p -2 -2	P $\bar{2}$ $\bar{2}$
26	P m c 21	p 2c -2	P 2_c $\bar{2}$
26:ba-c	P c m 21	p 2c -2c	P 2_c $\bar{2}_c$
26:cab	P 21 m a	p -2a 2a	P $\bar{2}_a$ 2_a
26:-cba	P 21 a m	p -2 2a	P $\bar{2}$ 2_a
26:bca	P b 21 m	p -2 -2b	P $\bar{2}$ $\bar{2}_b$
26:a-cb	P m 21 b	p -2b -2	P $\bar{2}_b$ $\bar{2}$
27	P c c 2	p 2 -2c	P 2 $\bar{2}_c$
27:cab	P 2 a a	p -2a 2	P $\bar{2}_a$ 2
27:bca	P b 2 b	p -2b -2b	P $\bar{2}_b$ $\bar{2}_b$
28	P m a 2	p 2 -2a	P 2 $\bar{2}_a$
28:ba-c	P b m 2	p 2 -2b	P 2 $\bar{2}_b$
28:cab	P 2 m b	p -2b 2	P $\bar{2}_b$ 2
28:-cba	P 2 c m	p -2c 2	P $\bar{2}_c$ 2
28:bca	P c 2 m	p -2c -2c	P $\bar{2}_c$ $\bar{2}_c$
28:a-cb	P m 2 a	p -2a -2a	P $\bar{2}_a$ $\bar{2}_a$
29	P c a 21	p 2c -2ac	P 2_c $\bar{2}_{ac}$
29:ba-c	P b c 21	p 2c -2b	P 2_c $\bar{2}_b$
29:cab	P 21 a b	p -2b 2a	P $\bar{2}_b$ 2_a
29:-cba	P 21 c a	p -2ac 2a	P $\bar{2}_{ac}$ 2_a
29:bca	P c 21 b	p -2bc -2c	P $\bar{2}_{bc}$ $\bar{2}_c$
29:a-cb	P b 21 a	p -2a -2ab	P $\bar{2}_a$ $\bar{2}_{ab}$
30	P n c 2	p 2 -2bc	P 2 $\bar{2}_{bc}$
30:ba-c	P c n 2	p 2 -2ac	P 2 $\bar{2}_{ac}$
30:cab	P 2 n a	p -2ac 2	P $\bar{2}_{ac}$ 2
30:-cba	P 2 a n	p -2ab 2	P $\bar{2}_{ab}$ 2
30:bca	P b 2 n	p -2ab -2ab	P $\bar{2}_{ab}$ $\bar{2}_{ab}$
30:a-cb	P n 2 b	p -2bc -2bc	P $\bar{2}_{bc}$ $\bar{2}_{bc}$
31	P m n 21	p 2ac -2	P 2_{ac} $\bar{2}$
31:ba-c	P n m 21	p 2bc -2bc	P 2_{bc} $\bar{2}_{bc}$
31:cab	P 21 m n	p -2ab 2ab	P $\bar{2}_{ab}$ 2_{ab}
31:-cba	P 21 n m	p -2 2ac	P $\bar{2}$ 2_{ac}
31:bca	P n 21 m	p -2 -2bc	P $\bar{2}$ $\bar{2}_{bc}$
31:a-cb	P m 21 n	p -2ab -2	P $\bar{2}_{ab}$ $\bar{2}$
32	P b a 2	p 2 -2ab	P 2 $\bar{2}_{ab}$
32:cab	P 2 c b	p -2bc 2	P $\bar{2}_{bc}$ 2
32:bca	P c 2 a	p -2ac -2ac	P $\bar{2}_{ac}$ $\bar{2}_{ac}$
33	P n a 21	p 2c -2n	P 2_c $\bar{2}_n$
33:ba-c	P b n 21	p 2c -2ab	P 2_c $\bar{2}_{ab}$
33:cab	P 21 n b	p -2bc 2a	P $\bar{2}_{bc}$ 2_a
33:-cba	P 21 c n	p -2n 2a	P $\bar{2}_n$ 2_a
33:bca	P c 21 n	p -2n -2ac	P $\bar{2}_n$ $\bar{2}_{ac}$
33:a-cb	P n 21 a	p -2ac -2n	P $\bar{2}_{ac}$ $\bar{2}_n$
34	P n n 2	p 2 -2n	P 2 $\bar{2}_n$
34:cab	P 2 n n	p -2n 2	P $\bar{2}_n$ 2
34:bca	P n 2 n	p -2n -2n	P $\bar{2}_n$ $\bar{2}_n$
35	C m m 2	c 2 -2	C 2 $\bar{2}$
35:cab	A 2 m m	a -2 2	A $\bar{2}$ 2
35:bca	B m 2 m	b -2 -2	B $\bar{2}$ $\bar{2}$
36	C m c 21	c 2c -2	C 2_c $\bar{2}$
36:ba-c	C c m 21	c 2c -2c	C 2_c $\bar{2}_c$
36:cab	A 21 m a	a -2a 2a	A $\bar{2}_a$ 2_a
36:-cba	A 21 a m	a -2 2a	A $\bar{2}$ 2_a
36:bca	B b 21 m	b -2 -2b	B $\bar{2}$ $\bar{2}_b$
36:a-cb	B m 21 b	b -2b -2	B $\bar{2}_b$ $\bar{2}$
37	C c c 2	c 2 -2c	C 2 $\bar{2}_c$
37:cab	A 2 a a	a -2a 2	A $\bar{2}_a$ 2
37:bca	B b 2 b	b -2b -2b	B $\bar{2}_b$ $\bar{2}_b$
38	A m m 2	a 2 -2	A 2 $\bar{2}$
38:ba-c	B m m 2	b 2 -2	B 2 $\bar{2}$
38:cab	B 2 m m	b -2 2	B $\bar{2}$ 2
38:-cba	C 2 m m	c -2 2	C $\bar{2}$ 2
38:bca	C m 2 m	c -2 -2	C $\bar{2}$ $\bar{2}$
38:a-cb	A m 2 m	a -2 -2	A $\bar{2}$ $\bar{2}$
39	A b m 2	a 2 -2b	A 2 $\bar{2}_b$
39:ba-c	B m a 2	b 2 -2a	B 2 $\bar{2}_a$
39:cab	B 2 c m	b -2a 2	B $\bar{2}_a$ 2
39:-cba	C 2 m b	c -2a 2	C $\bar{2}_a$ 2
39:bca	C m 2 a	c -2a -2a	C $\bar{2}_a$ $\bar{2}_a$
39:a-cb	A c 2 m	a -2b -2b	A $\bar{2}_b$ $\bar{2}_b$
40	A m a 2	a 2 -2a	A 2 $\bar{2}_a$
40:ba-c	B b m 2	b 2 -2b	B 2 $\bar{2}_b$
40:cab	B 2 m b	b -2b 2	B $\bar{2}_b$ 2
40:-cba	C 2 c m	c -2c 2	C $\bar{2}_c$ 2
40:bca	C c 2 m	c -2c -2c	C $\bar{2}_c$ $\bar{2}_c$
40:a-cb	A m 2 a	a -2a -2a	A $\bar{2}_a$ $\bar{2}_a$
41	A b a 2	a 2 -2ab	A 2 $\bar{2}_{ab}$
41:ba-c	B b a 2	b 2 -2ab	B 2 $\bar{2}_{ab}$
41:cab	B 2 c b	b -2ab 2	B $\bar{2}_{ab}$ 2
41:-cba	C 2 c b	c -2ac 2	C $\bar{2}_{ac}$ 2
41:bca	C c 2 a	c -2ac -2ac	C $\bar{2}_{ac}$ $\bar{2}_{ac}$
41:a-cb	A c 2 a	a -2ab -2ab	A $\bar{2}_{ab}$ $\bar{2}_{ab}$
42	F m m 2	f 2 -2	F 2 $\bar{2}$
42:cab	F 2 m m	f -2 2	F $\bar{2}$ 2
42:bca	F m 2 m	f -2 -2	F $\bar{2}$ $\bar{2}$
43	F d d 2	f 2 -2d	F 2 $\bar{2}_d$
43:cab	F 2 d d	f -2d 2	F $\bar{2}_d$ 2
43:bca	F d 2 d	f -2d -2d	F $\bar{2}_d$ $\bar{2}_d$
44	I m m 2	i 2 -2	I 2 $\bar{2}$
44:cab	I 2 m m	i -2 2	I $\bar{2}$ 2
44:bca	I m 2 m	i -2 -2	I $\bar{2}$ $\bar{2}$
45	I b a 2	i 2 -2c	I 2 $\bar{2}_c$
45:cab	I 2 c b	i -2a 2	I $\bar{2}_a$ 2
45:bca	I c 2 a	i -2b -2b	I $\bar{2}_b$ $\bar{2}_b$

Table A1.4.2.7. *Hall symbols* (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
46	I m a 2	i 2 -2a	I 2 $\bar{2}_a$
46:ba-c	I b m 2	i 2 -2b	I 2 $\bar{2}_b$
46:cab	I 2 m b	i -2b 2	I $\bar{2}_b$ 2
46:-cba	I 2 c m	i -2c 2	I $\bar{2}_c$ 2
46:bca	I c 2 m	i -2c -2c	I $\bar{2}_c$ $\bar{2}_c$
46:a-cb	I m 2 a	i -2a -2a	I $\bar{2}_a$ $\bar{2}_a$
47	P m m m	-p 2 2	$\bar{P}$ 2 2
48:1	P n n n:1	p 2 2 -1n	P 2 2 $\bar{1}_n$
48:2	P n n n:2	-p 2ab 2bc	$\bar{P}$ 2_{ab} 2_{bc}
49	P c c m	-p 2 2c	$\bar{P}$ 2 2_c
49:cab	P m a a	-p 2a 2	$\bar{P}$ 2_a 2
49:bca	P b m b	-p 2b 2b	$\bar{P}$ 2_b 2_b
50:1	P b a n:1	p 2 2 -1ab	P 2 2 $\bar{1}_{ab}$
50:2	P b a n:2	-p 2ab 2b	$\bar{P}$ 2_{ab} 2_b
50:1cab	P n c b:1	p 2 2 -1bc	P 2 2 $\bar{1}_{bc}$
50:2cab	P n c b:2	-p 2b 2bc	$\bar{P}$ 2_b 2_{bc}
50:1bca	P c n a:1	p 2 2 -1ac	P 2 2 $\bar{1}_{ac}$
50:2bca	P c n a:2	-p 2a 2c	$\bar{P}$ 2_a 2_c
51	P m m a	-p 2a 2a	$\bar{P}$ 2_a 2_a
51:ba-c	P m m b	-p 2b 2	$\bar{P}$ 2_b 2
51:cab	P b m m	-p 2 2b	$\bar{P}$ 2 2_b
51:-cba	P c m m	-p 2c 2c	$\bar{P}$ 2_c 2_c
51:bca	P m c m	-p 2c 2	$\bar{P}$ 2_c 2
51:a-cb	P m a m	-p 2 2a	$\bar{P}$ 2 2_a
52	P n n a	-p 2a 2bc	$\bar{P}$ 2_a 2_{bc}
52:ba-c	P n n b	-p 2b 2n	$\bar{P}$ 2_b 2_n
52:cab	P b n n	-p 2n 2b	$\bar{P}$ 2_n 2_b
52:-cba	P c n n	-p 2ab 2c	$\bar{P}$ 2_{ab} 2_c
52:bca	P n c n	-p 2ab 2n	$\bar{P}$ 2_{ab} 2_n
52:a-cb	P n a n	-p 2n 2bc	$\bar{P}$ 2_n 2_{bc}
53	P m n a	-p 2ac 2	$\bar{P}$ 2_{ac} 2
53:ba-c	P n m b	-p 2bc 2bc	$\bar{P}$ 2_{bc} 2_{bc}
53:cab	P b m n	-p 2ab 2ab	$\bar{P}$ 2_{ab} 2_{ab}
53:-cba	P c n m	-p 2 2ac	$\bar{P}$ 2 2_{ac}
53:bca	P n c m	-p 2 2bc	$\bar{P}$ 2 2_{bc}
53:a-cb	P m a n	-p 2ab 2	$\bar{P}$ 2_{ab} 2
54	P c c a	-p 2a 2ac	$\bar{P}$ 2_a 2_{ac}
54:ba-c	P c c b	-p 2b 2c	$\bar{P}$ 2_b 2_c
54:cab	P b a a	-p 2a 2b	$\bar{P}$ 2_a 2_b
54:-cba	P c a a	-p 2ac 2c	$\bar{P}$ 2_{ac} 2_c
54:bca	P b c b	-p 2bc 2b	$\bar{P}$ 2_{bc} 2_b
54:a-cb	P b a b	-p 2b 2ab	$\bar{P}$ 2_b 2_{ab}
55	P b a m	-p 2 2ab	$\bar{P}$ 2 2_{ab}
55:cab	P m c b	-p 2bc 2	$\bar{P}$ 2_{bc} 2
55:bca	P c m a	-p 2ac 2ac	$\bar{P}$ 2_{ac} 2_{ac}
56	P c c n	-p 2ab 2ac	$\bar{P}$ 2_{ab} 2_{ac}
56:cab	P n a a	-p 2ac 2bc	$\bar{P}$ 2_{ac} 2_{bc}
56:bca	P b n b	-p 2bc 2ab	$\bar{P}$ 2_{bc} 2_{ab}
57	P b c m	-p 2c 2b	$\bar{P}$ 2_c 2_b
57:ba-c	P c a m	-p 2c 2ac	$\bar{P}$ 2_c 2_{ac}
57:cab	P m c a	-p 2ac 2a	$\bar{P}$ 2_{ac} 2_a
57:-cba	P m a b	-p 2b 2a	$\bar{P}$ 2_b 2_a
57:bca	P b m a	-p 2a 2ab	$\bar{P}$ 2_a 2_{ab}
57:a-cb	P c m b	-p 2bc 2c	$\bar{P}$ 2_{bc} 2_c
58	P n n m	-p 2 2n	$\bar{P}$ 2 2_n
58:cab	P m n n	-p 2n 2	$\bar{P}$ 2_n 2

n:c	H–M entry	Hall entry	Hall symbol
58:bca	P n m n	-p 2n 2n	$\bar{P}$ 2_n 2_n
59:1	P m m n:1	p 2 2ab -1ab	P 2 2_{ab} $\bar{1}_{ab}$
59:2	P m m n:2	-p 2ab 2a	$\bar{P}$ 2_{ab} 2_a
59:1cab	P n m m:1	p 2bc 2 -1bc	P 2_{bc} 2 $\bar{1}_{bc}$
59:2cab	P n m m:2	-p 2c 2bc	$\bar{P}$ 2_c 2_{bc}
59:1bca	P m n m:1	p 2ac 2ac -1ac	P 2_{ac} 2_{ac} $\bar{1}_{ac}$
59:2bca	P m n m:2	-p 2c 2a	$\bar{P}$ 2_c 2_a
60	P b c n	-p 2n 2ab	$\bar{P}$ 2_n 2_{ab}
60:ba-c	P c a n	-p 2n 2c	$\bar{P}$ 2_n 2_c
60:cab	P n c a	-p 2a 2n	$\bar{P}$ 2_a 2_n
60:-cba	P n a b	-p 2bc 2n	$\bar{P}$ 2_{bc} 2_n
60:bca	P b n a	-p 2ac 2b	$\bar{P}$ 2_{ac} 2_b
60:a-cb	P c n b	-p 2b 2ac	$\bar{P}$ 2_b 2_{ac}
61	P b c a	-p 2ac 2ab	$\bar{P}$ 2_{ac} 2_{ab}
61:ba-c	P c a b	-p 2bc 2ac	$\bar{P}$ 2_{bc} 2_{ac}
62	P n m a	-p 2ac 2n	$\bar{P}$ 2_{ac} 2_n
62:ba-c	P m n b	-p 2bc 2a	$\bar{P}$ 2_{bc} 2_a
62:cab	P b n m	-p 2c 2ab	$\bar{P}$ 2_c 2_{ab}
62:-cba	P c m n	-p 2n 2ac	$\bar{P}$ 2_n 2_{ac}
62:bca	P m c n	-p 2n 2a	$\bar{P}$ 2_n 2_a
62:a-cb	P n a m	-p 2c 2n	$\bar{P}$ 2_c 2_n
63	C m c m	-c 2c 2	$\bar{C}$ 2_c 2
63:ba-c	C c m m	-c 2c 2c	$\bar{C}$ 2_c 2_c
63:cab	A m m a	-a 2a 2a	$\bar{A}$ 2_a 2_a
63:-cba	A m a m	-a 2 2a	$\bar{A}$ 2 2_a
63:bca	B b m m	-b 2 2b	$\bar{B}$ 2 2_b
63:a-cb	B m m b	-b 2b 2	$\bar{B}$ 2_b 2
64	C m c a	-c 2ac 2	$\bar{C}$ 2_{ac} 2
64:ba-c	C c m b	-c 2ac 2ac	$\bar{C}$ 2_{ac} 2_{ac}
64:cab	A b m a	-a 2ab 2ab	$\bar{A}$ 2_{ab} 2_{ab}
64:-cba	A c a m	-a 2 2ab	$\bar{A}$ 2 2_{ab}
64:bca	B b c m	-b 2 2ab	$\bar{B}$ 2 2_{ab}
64:a-cb	B m a b	-b 2ab 2	$\bar{B}$ 2_{ab} 2
65	C m m m	-c 2 2	$\bar{C}$ 2 2
65:cab	A m m m	-a 2 2	$\bar{A}$ 2 2
65:bca	B m m m	-b 2 2	$\bar{B}$ 2 2
66	C c c m	-c 2 2c	$\bar{C}$ 2 2_c
66:cab	A m a a	-a 2a 2	$\bar{A}$ 2_a 2
66:bca	B b m b	-b 2b 2b	$\bar{B}$ 2_b 2_b
67	C m m a	-c 2a 2	$\bar{C}$ 2_a 2
67:ba-c	C m m b	-c 2a 2a	$\bar{C}$ 2_a 2_a
67:cab	A b m m	-a 2b 2b	$\bar{A}$ 2_b 2_b
67:-cba	A c m m	-a 2 2b	$\bar{A}$ 2 2_b
67:bca	B m c m	-b 2 2a	$\bar{B}$ 2 2_a
67:a-cb	B m a m	-b 2a 2	$\bar{B}$ 2_a 2
68:1	C c c a:1	c 2 2 -1ac	C 2 2 $\bar{1}_{ac}$
68:2	C c c a:2	-c 2a 2ac	$\bar{C}$ 2_a 2_{ac}
68:1ba-c	C c c b:1	c 2 2 -1ac	C 2 2 $\bar{1}_{ac}$
68:2ba-c	C c c b:2	-c 2a 2c	$\bar{C}$ 2_a 2_c
68:1cab	A b a a:1	a 2 2 -1ab	A 2 2 $\bar{1}_{ab}$
68:2cab	A b a a:2	-a 2a 2b	$\bar{A}$ 2_a 2_b
68:1-cba	A c a a:1	a 2 2 -1ab	A 2 2 $\bar{1}_{ab}$
68:2-cba	A c a a:2	-a 2ab 2b	$\bar{A}$ 2_{ab} 2_b
68:1bca	B b c b:1	b 2 2 -1ab	B 2 2 $\bar{1}_{ab}$
68:2bca	B b c b:2	-b 2ab 2b	$\bar{B}$ 2_{ab} 2_b
68:1a-cb	B b a b:1	b 2 2 -1ab	B 2 2 $\bar{1}_{ab}$

Table A1.4.2.7. *Hall symbols* (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
68:2a-cb	B b a b:2	-b 2b 2ab	$\bar{B}\ 2_{b}\ 2_{ab}$
69	F m m m	-f 2 2	$\bar{F}\ 2\ 2$
70:1	F d d d:1	f 2 2 -1d	$F\ 2\ 2\ \bar{1}_{d}$
70:2	F d d d:2	-f 2uv 2vw	$\bar{F}\ 2_{uv}\ 2_{vw}$
71	I m m m	-i 2 2	$\bar{I}\ 2\ 2$
72	I b a m	-i 2 2c	$\bar{I}\ 2\ 2_{c}$
72:cab	I m c b	-i 2a 2	$\bar{I}\ 2_{a}\ 2$
72:bca	I c m a	-i 2b 2b	$\bar{I}\ 2_{b}\ 2_{b}$
73	I b c a	-i 2b 2c	$\bar{I}\ 2_{b}\ 2_{c}$
73:ba-c	I c a b	-i 2a 2b	$\bar{I}\ 2_{a}\ 2_{b}$
74	I m m a	-i 2b 2	$\bar{I}\ 2_{b}\ 2$
74:ba-c	I m m b	-i 2a 2a	$\bar{I}\ 2_{a}\ 2_{a}$
74:cab	I b m m	-i 2c 2c	$\bar{I}\ 2_{c}\ 2_{c}$
74:-cba	I c m m	-i 2 2b	$\bar{I}\ 2\ 2_{b}$
74:bca	I m c m	-i 2 2a	$\bar{I}\ 2\ 2_{a}$
74:a-cb	I m a m	-i 2c 2	$\bar{I}\ 2_{c}\ 2$
75	P 4	p 4	$P\ 4$
76	P 41	p 4w	$P\ 4_{w}$
77	P 42	p 4c	$P\ 4_{c}$
78	P 43	p 4cw	$P\ 4_{cw}$
79	I 4	i 4	$I\ 4$
80	I 41	i 4bw	$I\ 4_{bw}$
81	P -4	p -4	$P\ \bar{4}$
82	I -4	i -4	$I\ \bar{4}$
83	P 4/m	-p 4	$\bar{P}\ 4$
84	P 42/m	-p 4c	$\bar{P}\ 4_{c}$
85:1	P 4/n:1	p 4ab -1ab	$P\ 4_{ab}\ \bar{1}_{ab}$
85:2	P 4/n:2	-p 4a	$\bar{P}\ 4_{a}$
86:1	P 42/n:1	p 4n -1n	$P\ 4_{n}\ \bar{1}_{n}$
86:2	P 42/n:2	-p 4bc	$\bar{P}\ 4_{bc}$
87	I 4/m	-i 4	$\bar{I}\ 4$
88:1	I 41/a:1	i 4bw -1bw	$I\ 4_{bw}\ \bar{1}_{bw}$
88:2	I 41/a:2	-i 4ad	$\bar{I}\ 4_{ad}$
89	P 4 2 2	p 4 2	$P\ 4\ 2$
90	P 4 21 2	p 4ab 2ab	$P\ 4_{ab}\ 2_{ab}$
91	P 41 2 2	p 4w 2c	$P\ 4_{w}\ 2_{c}$
92	P 41 21 2	p 4abw 2nw	$P4_{abw}2_{nw}$
93	P 42 2 2	p 4c 2	$P\ 4_{c}\ 2$
94	P 42 21 2	p 4n 2n	$P\ 4_{n}\ 2_{n}$
95	P 43 2 2	p 4cw 2c	$P\ 4_{cw}\ 2_{c}$
96	P 43 21 2	p 4nw 2abw	$P\ 4_{nw}\ 2_{abw}$
97	I 4 2 2	i 4 2	$I\ 4\ 2$
98	I 41 2 2	i 4bw 2bw	$I\ 4_{bw}\ 2_{bw}$
99	P 4 m m	p 4 -2	$P\ 4\ \bar{2}$
100	P 4 b m	p 4 -2ab	$P\ 4\ \bar{2}_{ab}$
101	P 42 c m	p 4c -2c	$P\ 4_{c}\ \bar{2}_{c}$
102	P 42 n m	p 4n -2n	$P\ 4_{n}\ \bar{2}_{n}$
103	P 4 c c	p 4 -2c	$P\ 4\ \bar{2}_{c}$
104	P 4 n c	p 4 -2n	$P\ 4\ \bar{2}_{n}$
105	P 42 m c	p 4c -2	$P\ 4_{c}\ \bar{2}$
106	P 42 b c	p 4c -2ab	$P\ 4_{c}\ \bar{2}_{ab}$
107	I 4 m m	i 4 -2	$I\ 4\ \bar{2}$
108	I 4 c m	i 4 -2c	$I\ 4\ \bar{2}_{c}$
109	I 41 m d	i 4bw -2	$I\ 4_{bw}\ \bar{2}$
110	I 41 c d	i 4bw -2c	$I\ 4_{bw}\ \bar{2}_{c}$
111	P -4 2 m	p -4 2	$P\ \bar{4}\ 2$
112	P -4 2 c	p -4 2c	$P\ \bar{4}\ 2_{c}$
113	P -4 21 m	p -4 2ab	$P\ \bar{4}\ 2_{ab}$
114	P -4 21 c	p -4 2n	$P\ \bar{4}\ 2_{n}$
115	P -4 m 2	p -4 -2	$P\ \bar{4}\ \bar{2}$
116	P -4 c 2	p -4 -2c	$P\ \bar{4}\ \bar{2}_{c}$
117	P -4 b 2	p -4 -2ab	$P\ \bar{4}\ \bar{2}_{ab}$
118	P -4 n 2	p -4 -2n	$P\ \bar{4}\ \bar{2}_{n}$
119	I -4 m 2	i -4 -2	$I\ \bar{4}\ \bar{2}$
120	I -4 c 2	i -4 -2c	$I\ \bar{4}\ \bar{2}_{c}$
121	I -4 2 m	i -4 2	$I\ \bar{4}\ 2$
122	I -4 2 d	i -4 2bw	$I\ \bar{4}\ 2_{bw}$
123	P 4/m m m	-p 4 2	$\bar{P}\ 4\ 2$
124	P 4/m c c	-p 4 2c	$\bar{P}\ 4\ 2_{c}$
125:1	P 4/n b m:1	p 4 2 -1ab	$P\ 4\ 2\ \bar{1}_{ab}$
125:2	P 4/n b m:2	-p 4a 2b	$\bar{P}\ 4_{a}\ 2_{b}$
126:1	P 4/n n c:1	p 4 2 -1n	$P\ 4\ 2\ \bar{1}_{n}$
126:2	P 4/n n c:2	-p 4a 2bc	$\bar{P}\ 4_{a}\ 2_{bc}$
127	P 4/m b m	-p 4 2ab	$\bar{P}\ 4\ 2_{ab}$
128	P 4/m n c	-p 4 2n	$\bar{P}\ 4\ 2_{n}$
129:1	P 4/n m m:1	p 4ab 2ab -1ab	$P\ 4_{ab}\ 2_{ab}\ \bar{1}_{ab}$
129:2	P 4/n m m:2	-p 4a 2a	$\bar{P}\ 4_{a}\ 2_{a}$
130:1	P 4/n c c:1	p 4ab 2n -1ab	$P\ 4_{ab}\ 2_{n}\ \bar{1}_{ab}$
130:2	P 4/n c c:2	-p 4a 2ac	$\bar{P}\ 4_{a}\ 2_{ac}$
131	P 42/m m c	-p 4c 2	$\bar{P}\ 4_{c}\ 2$
132	P 42/m c m	-p 4c 2c	$\bar{P}\ 4_{c}\ 2_{c}$
133:1	P 42/n b c:1	p 4n 2c -1n	$P\ 4_{n}\ 2_{c}\ \bar{1}_{n}$
133:2	P 42/n b c:2	-p 4ac 2b	$\bar{P}\ 4_{ac}\ 2_{b}$
134:1	P 42/n n m:1	p 4n 2 -1n	$P\ 4_{n}\ 2\ \bar{1}_{n}$
134:2	P 42/n n m:2	-p 4ac 2bc	$\bar{P}\ 4_{ac}\ 2_{bc}$
135	P 42/m b c	-p 4c 2ab	$\bar{P}\ 4_{c}\ 2_{ab}$
136	P 42/m n m	-p 4n 2n	$\bar{P}\ 4_{n}\ 2_{n}$
137:1	P 42/n m c:1	p 4n 2n -1n	$P\ 4_{n}\ 2_{n}\ \bar{1}_{n}$
137:2	P 42/n m c:2	-p 4ac 2a	$\bar{P}\ 4_{ac}\ 2_{a}$
138:1	P 42/n c m:1	p 4n 2ab -1n	$P\ 4_{n}\ 2_{ab}\ \bar{1}_{n}$
138:2	P 42/n c m:2	-p 4ac 2ac	$\bar{P}\ 4_{ac}\ 2_{ac}$
139	I 4/m m m	-i 4 2	$\bar{I}\ 4\ 2$
140	I 4/m c m	-i 4 2c	$\bar{I}\ 4\ 2_{c}$
141:1	I 41/a m d:1	i 4bw 2bw -1bw	$I\ 4_{bw}\ 2_{bw}\ \bar{1}_{bw}$
141:2	I 41/a m d:2	-i 4bd 2	$\bar{I}\ 4_{bd}\ 2$
142:1	I 41/a c d:1	i 4bw 2aw -1bw	$I\ 4_{bw}\ 2_{aw}\ \bar{1}_{bw}$
142:2	I 41/a c d:2	-i 4bd 2c	$\bar{I}\ 4_{bd}\ 2_{c}$
143	P 3	p 3	$P\ 3$
144	P 31	p 31	$P\ 3_{1}$
145	P 32	p 32	$P\ 3_{2}$
146:h	R 3:h	r 3	$R\ 3$
146:r	R 3:r	p 3*	$P\ 3*$
147	P -3	-p 3	$\bar{P}\ 3$
148:h	R -3:h	-r 3	$\bar{R}\ 3$
148:r	R -3:r	-p 3*	$\bar{P}\ 3*$
149	P 3 1 2	p 3 2	$P\ 3\ 2$
150	P 3 2 1	p 3 2"	$P\ 3\ 2''$
151	P 31 1 2	p 31 2 (0 0 4)	$P\ 3_{1}\ 2\ (0\ 0\ 4)$
152	P 31 2 1	p 31 2"	$P\ 3_{1}\ 2''$
153	P 32 1 2	p 32 2 (0 0 2)	$P\ 3_{2}\ 2\ (0\ 0\ 2)$
154	P 32 2 1	p 32 2"	$P\ 3_{2}\ 2''$
155:h	R 3 2:h	r 3 2"	$R\ 3\ 2''$

Table A1.4.2.7. *Hall symbols* (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
155:r	R 3 2:r	p 3* 2	P 3* 2
156	P 3 m 1	p 3 -2"	P 3 $\bar{2}''$
157	P 3 1 m	p 3 -2	P 3 $\bar{2}$
158	P 3 c 1	p 3 -2"c	P 3 $\bar{2}''_c$
159	P 3 1 c	p 3 -2c	P 3 $\bar{2}_c$
160:h	R 3 m:h	r 3 -2"	R 3 $\bar{2}''$
160:r	R 3 m:r	p 3* -2	P 3* $\bar{2}$
161:h	R 3 c:h	r 3 -2"c	R 3 $\bar{2}''_c$
161:r	R 3 c:r	p 3* -2n	P 3* $\bar{2}_n$
162	P -3 1 m	-p 3 2	$\bar{P}$ 3 2
163	P -3 1 c	-p 3 2c	$\bar{P}$ 3 2_c
164	P -3 m 1	-p 3 2"	$\bar{P}$ 3 2"
165	P -3 c 1	-p 3 2"c	$\bar{P}$ 3 $2''_c$
166:h	R -3 m:h	-r 3 2"	$\bar{R}$ 3 2"
166:r	R -3 m:r	-p 3* 2	$\bar{P}$ 3* 2
167:h	R -3 c:h	-r 3 2"c	$\bar{R}$ 3 $2''_c$
167:r	R -3 c:r	-p 3* 2n	$\bar{P}$ 3* 2_n
168	P 6	p 6	P 6
169	P 61	p 61	P 6_1
170	P 65	p 65	P 6_5
171	P 62	p 62	P 6_2
172	P 64	p 64	P 6_4
173	P 63	p 6c	P 6_c
174	P -6	p -6	P $\bar{6}$
175	P 6/m	-p 6	$\bar{P}$ 6
176	P 63/m	-p 6c	$\bar{P}$ 6_c
177	P 6 2 2	p 6 2	P 6 2
178	P 61 2 2	p 61 2 (0 0 5)	P 6_1 2 (0 0 5)
179	P 65 2 2	p 65 2 (0 0 1)	P 6_5 2 (0 0 1)
180	P 62 2 2	p 62 2 (0 0 4)	P 6_2 2 (0 0 4)
181	P 64 2 2	p 64 2 (0 0 2)	P 6_4 2 (0 0 2)
182	P 63 2 2	p 6c 2c	P 6_c 2_c
183	P 6 m m	p 6 -2	P 6 $\bar{2}$
184	P 6 c c	p 6 -2c	P 6 $\bar{2}_c$
185	P 63 c m	p 6c -2	P 6_c $\bar{2}$
186	P 63 m c	p 6c -2c	P 6_c $\bar{2}_c$
187	P -6 m 2	p -6 2	P $\bar{6}$ 2
188	P -6 c 2	p -6c 2	P $\bar{6}_c$ 2
189	P -6 2 m	p -6 -2	P $\bar{6}$ $\bar{2}$
190	P -6 2 c	p -6c -2c	P $\bar{6}_c$ $\bar{2}_c$
191	P 6/m m m	-p 6 2	$\bar{P}$ 6 2
192	P 6/m c c	-p 6 2c	$\bar{P}$ 6 2_c
193	P 63/m c m	-p 6c 2	$\bar{P}$ 6_c 2
194	P 63/m m c	-p 6c 2c	$\bar{P}$ 6_c 2_c
195	P 2 3	p 2 2 3	P 2 2 3
196	F 2 3	f 2 2 3	F 2 2 3
197	I 2 3	i 2 2 3	I 2 2 3
198	P 21 3	p 2ac 2ab 3	P 2_{ac} 2_{ab} 3
199	I 21 3	i 2b 2c 3	I 2_b 2_c 3
200	P m -3	-p 2 2 3	$\bar{P}$ 2 2 3
201:1	P n -3:1	p 2 2 3 -1n	P 2 2 3 $\bar{1}_n$
201:2	P n -3:2	-p 2ab 2bc 3	$\bar{P}$ 2_{ab} 2_{bc} 3
202	F m -3	-f 2 2 3	$\bar{F}$ 2 2 3
203:1	F d -3:1	f 2 2 3 -1d	F 2 2 3 $\bar{1}_d$
203:2	F d -3:2	-f 2uv 2vw 3	$\bar{F}$ 2_{uv} 2_{vw} 3
204	I m -3	-i 2 2 3	$\bar{I}$ 2 2 3
205	P a -3	-p 2ac 2ab 3	$\bar{P}$ 2_{ac} 2_{ab} 3
206	I a -3	-i 2b 2c 3	$\bar{I}$ 2_b 2_c 3
207	P 4 3 2	p 4 2 3	P 4 2 3
208	P 42 3 2	p 4n 2 3	P 4_n 2 3
209	F 4 3 2	f 4 2 3	F 4 2 3
210	F 41 3 2	f 4d 2 3	F 4_d 2 3
211	I 4 3 2	i 4 2 3	I 4 2 3
212	P 43 3 2	p 4acd 2ab 3	P 4_{acd} 2_{ab} 3
213	P 41 3 2	p 4bd 2ab 3	P 4_{bd} 2_{ab} 3
214	I 41 3 2	i 4bd 2c 3	I 4_{bd} 2_c 3
215	P -4 3 m	p -4 2 3	P $\bar{4}$ 2 3
216	F -4 3 m	f -4 2 3	F $\bar{4}$ 2 3
217	I -4 3 m	i -4 2 3	I $\bar{4}$ 2 3
218	P -4 3 n	p -4n 2 3	P $\bar{4}_n$ 2 3
219	F -4 3 c	f -4a 2 3	F $\bar{4}_a$ 2 3
220	I -4 3 d	i -4bd 2c 3	I $\bar{4}_{bd}$ 2_c 3
221	P m -3 m	-p 4 2 3	$\bar{P}$ 4 2 3
222:1	P n -3 n:1	p 4 2 3 -1n	P 4 2 3 $\bar{1}_n$
222:2	P n -3 n:2	-p 4a 2bc 3	$\bar{P}$ 4_a 2_{bc} 3
223	P m -3 n	-p 4n 2 3	$\bar{P}$ 4_n 2 3
224:1	P n -3 m:1	p 4n 2 3 -1n	P 4_n 2 3 $\bar{1}_n$
224:2	P n -3 m:2	-p 4bc 2bc 3	$\bar{P}$ 4_{bc} 2_{bc} 3
225	F m -3 m	-f 4 2 3	$\bar{F}$ 4 2 3
226	F m -3 c	-f 4a 2 3	$\bar{F}$ 4_a 2 3
227:1	F d -3 m:1	f 4d 2 3 -1d	F 4_d 2 3 $\bar{1}_d$
227:2	F d -3 m:2	-f 4vw 2vw 3	$\bar{F}$ 4_{vw} 2_{vw} 3
228:1	F d -3 c:1	f 4d 2 3 -1ad	F 4_d 2 3 $\bar{1}_{ad}$
228:2	F d -3 c:2	-f 4ud 2vw 3	$\bar{F}$ 4_{ud} 2_{vw} 3
229	I m -3 m	-i 4 2 3	$\bar{I}$ 4 2 3
230	I a -3 d	-i 4bd 2c 3	$\bar{I}$ 4_{bd} 2_c 3

The codes appended to the space-group numbers listed in the first column identify the relationship between the symmetry elements and the crystal cell. Where no code is given the first choice listed below applies.

Monoclinic. Code = <*unique axis*><*cell choice*>: unique axis choices [*cf. IT* A (1983) Table 4.3.1] b, -b, c, -c, a, -a; cell choices [*cf. IT* A (1983) Table 4.3.1] 1, 2, 3.

Orthorhombic. Code = <*origin choice*><*setting*>: origin choices 1, 2; setting choices [*cf. IT* A (1983) Table 4.3.1] abc, ba-c, cab, -cba, bca, a-cb.

Tetragonal, cubic. Code = <*origin choice*>: origin choices 1, 2.

Trigonal. Code = <*cell choice*>: cell choices h (hexagonal), r (rhombohedral).

Appendix 1.4.3.

Structure-factor tables

Table A1.4.3.1. *Plane groups*

The symbols appearing in this table are explained in Section 1.4.3 and in Tables A1.4.3.3 (monoclinic), A1.4.3.5 (tetragonal) and A1.4.3.6 (trigonal and hexagonal).

System	No.	Symbol	Parity	A	B
Oblique	1	$p1$		$c(hk)$	$s(hk)$
	2	$p2$		$2c(hk)$	0
Rectangular	3	pm		$2c(hx)c(ky)$	$2c(hx)s(ky)$
	4	pg	$k = 2n$	$2c(hx)c(ky)$	$2c(hx)s(ky)$
			$k = 2n+1$	$-2s(hx)s(ky)$	$2s(hx)c(ky)$
	5	cm		$4c(hx)c(ky)$	$4c(hx)s(ky)$
	6	$p2mm$		$4c(hx)c(ky)$	0
	7	$p2mg$	$h = 2n$	$4c(hx)c(ky)$	0
			$h = 2n+1$	$-4s(hx)s(ky)$	0
	8	$p2gg$	$h+k = 2n$	$4c(hx)c(ky)$	0
			$h+k = 2n+1$	$-4s(hx)s(ky)$	0
	9	$c2mm$		$8c(hx)c(ky)$	0
Square	10	$p4$		$2[P(cc) - M(ss)]$	0
	11	$p4mm$		$4P(cc)$	0
	12	$p4gm$	$h+k = 2n$	$4P(cc)$	0
			$h+k = 2n+1$	$-4M(ss)$	0
Hexagonal	13	$p3$		$C(hki)$	$S(hki)$
	14	$p3m1$		$PH(cc)$	$MH(ss)$
	15	$p31m$		$PH(cc)$	$PH(ss)$
	16	$p6$		$2C(hki)$	0
	17	$p6mm$		$2PH(cc)$	0

Table A1.4.3.2. *Triclinic space groups*

For the definition of the triple products ccc, csc *etc*., see Table A1.4.3.4.

$P1$ [No. 1]

hkl	A	B
All	$\cos 2\pi(hx+ky+lz) = \text{ccc} - \text{css} - \text{scs} - \text{ssc}$	$\sin 2\pi(hx+ky+lz) = \text{scc} + \text{csc} + \text{ccs} - \text{sss}$

$P\bar{1}$ [No. 2]

hkl	A	B
All	$2(\text{ccc} - \text{css} - \text{scs} - \text{ssc})$	0

Table A1.4.3.3. *Monoclinic space groups*

Each expression for *A* or *B* in the monoclinic system and for the space-group settings chosen in *IT* A is represented in terms of one of the following symbols:

$$\begin{aligned} \mathrm{c}(hl)\mathrm{c}(ky) &= \cos[2\pi(hx+lz)]\cos(2\pi ky), & \mathrm{c}(hk)\mathrm{c}(lz) &= \cos[2\pi(hx+ky)]\cos(2\pi lz),\\ \mathrm{c}(hl)\mathrm{s}(ky) &= \cos[2\pi(hx+lz)]\sin(2\pi ky), & \mathrm{c}(hk)\mathrm{s}(lz) &= \cos[2\pi(hx+ky)]\sin(2\pi lz),\\ \mathrm{s}(hl)\mathrm{c}(ky) &= \sin[2\pi(hx+lz)]\cos(2\pi ky), & \mathrm{s}(hk)\mathrm{c}(lz) &= \sin[2\pi(hx+ky)]\cos(2\pi lz),\\ \mathrm{s}(hl)\mathrm{s}(ky) &= \sin[2\pi(hx+lz)]\sin(2\pi ky), & \mathrm{s}(hk)\mathrm{s}(lz) &= \sin[2\pi(hx+ky)]\sin(2\pi lz), \end{aligned} \qquad \text{(A1.4.3.1)}$$

where the left-hand column of expressions corresponds to space-group representations in the second setting, with *b* taken as the unique axis, and the right-hand column corresponds to representations in the first setting, with *c* taken as the unique axis.

The lattice types in this table are *P*, *A*, *B*, *C* and *I*, and are all explicit in the full space-group symbol only (see below). Note that s(*hl*), s(*hk*), s(*ky*) and s(*lz*) are zero for *h* = *l* = 0, *h* = *k* = 0, *k* = 0 and *l* = 0, respectively.

No.	Group symbol		Parity	*A*	*B*	Unique axis
	Short	Full				
3	*P*2	*P*121		2c(*hl*)c(*ky*)	2c(*hl*)s(*ky*)	*b*
3	*P*2	*P*112		2c(*hk*)c(*lz*)	2c(*hk*)s(*lz*)	*c*
4	$P2_1$	$P12_11$	$k = 2n$	2c(*hl*)c(*ky*)	2c(*hl*)s(*ky*)	*b*
			$k = 2n + 1$	−2s(*hl*)s(*ky*)	2s(*hl*)c(*ky*)	
4	$P2_1$	$P112_1$	$l = 2n$	2c(*hk*)c(*lz*)	2c(*hk*)s(*lz*)	*c*
			$l = 2n + 1$	−2s(*hk*)s(*lz*)	2s(*hk*)c(*lz*)	
5	*C*2	*C*121		4c(*hl*)c(*ky*)	4c(*hl*)s(*ky*)	*b*
5	*C*2	*A*121		4c(*hl*)c(*ky*)	4c(*hl*)s(*ky*)	*b*
5	*C*2	*I*121		4c(*hl*)c(*ky*)	4c(*hl*)s(*ky*)	*b*
5	*C*2	*A*112		4c(*hk*)c(*lz*)	4c(*hk*)s(*lz*)	*c*
5	*C*2	*B*112		4c(*hk*)c(*lz*)	4c(*hk*)s(*lz*)	*c*
5	*C*2	*I*112		4c(*hk*)c(*lz*)	4c(*hk*)s(*lz*)	*c*
6	*Pm*	*P*1*m*1		2c(*hl*)c(*ky*)	2s(*hl*)c(*ky*)	*b*
6	*Pm*	*P*11*m*		2c(*hk*)c(*lz*)	2s(*hk*)c(*lz*)	*c*
7	*Pc*	*P*1*c*1	$l = 2n$	2c(*hl*)c(*ky*)	2s(*hl*)c(*ky*)	*b*
			$l = 2n + 1$	−2s(*hl*)s(*ky*)	2c(*hl*)s(*ky*)	
7	*Pc*	*P*1*n*1	$h + l = 2n$	2c(*hl*)c(*ky*)	2s(*hl*)c(*ky*)	*b*
			$h + l = 2n + 1$	−2s(*hl*)s(*ky*)	2c(*hl*)s(*ky*)	
7	*Pc*	*P*1*a*1	$h = 2n$	2c(*hl*)c(*ky*)	2s(*hl*)c(*ky*)	*b*
			$h = 2n + 1$	−2s(*hl*)s(*ky*)	2c(*hl*)s(*ky*)	
7	*Pc*	*P*11*a*	$h = 2n$	2c(*hk*)c(*lz*)	2s(*hk*)c(*lz*)	*c*
			$h = 2n + 1$	−2s(*hk*)s(*lz*)	2c(*hk*)s(*lz*)	
7	*Pc*	*P*11*n*	$h + k = 2n$	2c(*hk*)c(*lz*)	2s(*hk*)c(*lz*)	*c*
			$h + k = 2n + 1$	−2s(*hk*)s(*lz*)	2c(*hk*)s(*lz*)	
7	*Pc*	*P*11*b*	$k = 2n$	2c(*hk*)c(*lz*)	2s(*hk*)c(*lz*)	*c*
			$k = 2n + 1$	−2s(*hk*)s(*lz*)	2c(*hk*)s(*lz*)	
8	*Cm*	*C*1*m*1		4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
8	*Cm*	*A*1*m*1		4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
8	*Cm*	*I*1*m*1		4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
8	*Cm*	*A*11*m*		4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
8	*Cm*	*B*11*m*		4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
8	*Cm*	*I*11*m*		4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
9	*Cc*	*C*1*c*1	$l = 2n$	4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
			$l = 2n + 1$	−4s(*hl*)s(*ky*)	4c(*hl*)s(*ky*)	
9	*Cc*	*A*1*n*1	$h + l = 2n$	4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
			$h + l = 2n + 1$	−4s(*hl*)s(*ky*)	4c(*hl*)s(*ky*)	
9	*Cc*	*I*1*a*1	$h = 2n$	4c(*hl*)c(*ky*)	4s(*hl*)c(*ky*)	*b*
			$h = 2n + 1$	−4s(*hl*)s(*ky*)	4c(*hl*)s(*ky*)	
9	*Cc*	*A*11*a*	$h = 2n$	4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
			$h = 2n + 1$	−4s(*hk*)s(*lz*)	4c(*hk*)s(*lz*)	
9	*Cc*	*B*11*n*	$h + k = 2n$	4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
			$h + k = 2n + 1$	−4s(*hk*)s(*lz*)	4c(*hk*)s(*lz*)	
9	*Cc*	*I*11*b*	$k = 2n$	4c(*hk*)c(*lz*)	4s(*hk*)c(*lz*)	*c*
			$k = 2n + 1$	−4s(*hk*)s(*lz*)	4c(*hk*)s(*lz*)	
10	*P*2/*m*	*P*12/*m*1		4c(*hl*)c(*ky*)	0	*b*

Table A1.4.3.3. *Monoclinic space groups* (*cont.*)

No.	Group symbol: Short	Group symbol: Full	Parity	A	B	Unique axis
10	$P2/m$	$P112/m$		$4c(hk)c(lz)$	0	c
11	$P2_1/m$	$P12_1/m1$	$k=2n$	$4c(hl)c(ky)$	0	b
			$k=2n+1$	$-4s(hl)s(ky)$	0	
11	$P2_1/m$	$P112_1/m$	$l=2n$	$4c(hk)c(lz)$	0	c
			$l=2n+1$	$-4s(hk)s(lz)$	0	
12	$C2/m$	$C12/m1$		$8c(hl)c(ky)$	0	b
12	$C2/m$	$A12/m1$		$8c(hl)c(ky)$	0	b
12	$C2/m$	$I12/m1$		$8c(hl)c(ky)$	0	b
12	$C2/m$	$A112/m$		$8c(hk)c(lz)$	0	c
12	$C2/m$	$B112/m$		$8c(hk)c(lz)$	0	c
12	$C2/m$	$I112/m$		$8c(hk)c(lz)$	0	c
13	$P2/c$	$P12/c1$	$l=2n$	$4c(hl)c(ky)$	0	b
			$l=2n+1$	$-4s(hl)s(ky)$	0	
13	$P2/c$	$P12/n1$	$h+l=2n$	$4c(hl)c(ky)$	0	b
			$h+l=2n+1$	$-4s(hl)s(ky)$	0	
13	$P2/c$	$P12/a1$	$h=2n$	$4c(hl)c(ky)$	0	b
			$h=2n+1$	$-4s(hl)s(ky)$	0	
13	$P2/c$	$P112/a$	$h=2n$	$4c(hk)c(lz)$	0	c
			$h=2n+1$	$-4s(hk)s(lz)$	0	
13	$P2/c$	$P112/n$	$h+k=2n$	$4c(hk)c(lz)$	0	c
			$h+k=2n+1$	$-4s(hk)s(lz)$	0	
13	$P2/c$	$P112/b$	$k=2n$	$4c(hk)c(lz)$	0	c
			$k=2n+1$	$-4s(hk)s(lz)$	0	
14	$P2_1/c$	$P12_1/c1$	$k+l=2n$	$4c(hl)c(ky)$	0	b
			$k+l=2n+1$	$-4s(hl)s(ky)$	0	
14	$P2_1/c$	$P12_1/n1$	$h+k+l=2n$	$4c(hl)c(ky)$	0	b
			$h+k+l=2n+1$	$-4s(hl)s(ky)$	0	
14	$P2_1/c$	$P12_1/a1$	$h+k=2n$	$4c(hl)c(ky)$	0	b
			$h+k=2n+1$	$-4s(hl)s(ky)$	0	
14	$P2_1/c$	$P112_1/a$	$h+l=2n$	$4c(hk)c(lz)$	0	c
			$h+l=2n+1$	$-4s(hk)s(lz)$	0	
14	$P2_1/c$	$P112_1/n$	$h+k+l=2n$	$4c(hk)c(lz)$	0	c
			$h+k+l=2n+1$	$-4s(hk)s(lz)$	0	
14	$P2_1/c$	$P112_1/b$	$k+l=2n$	$4c(hk)c(lz)$	0	c
			$k+l=2n+1$	$-4s(hk)s(lz)$	0	
15	$C2/c$	$C12/c1$	$l=2n$	$8c(hl)c(ky)$	0	b
			$l=2n+1$	$-8s(hl)s(ky)$	0	
15	$C2/c$	$A12/n1$	$h+l=2n$	$8c(hl)c(ky)$	0	b
			$h+l=2n+1$	$-8s(hl)s(ky)$	0	
15	$C2/c$	$I12/a1$	$h=2n$	$8c(hl)c(ky)$	0	b
			$h=2n+1$	$-8s(hl)s(ky)$	0	
15	$C2/c$	$A112/a$	$h=2n$	$8c(hk)c(lz)$	0	c
			$h=2n+1$	$-8s(hk)s(lz)$	0	
15	$C2/c$	$B112/n$	$h+k=2n$	$8c(hk)c(lz)$	0	c
			$h+k=2n+1$	$-8s(hk)s(lz)$	0	
15	$C2/c$	$I112/b$	$k=2n$	$8c(hk)c(lz)$	0	c
			$k=2n+1$	$-8s(hk)s(lz)$	0	

Table A1.4.3.4. *Orthorhombic space groups*

The expressions for *A* and *B* for the orthorhombic space groups in their standard settings [as in *IT* A (1983)] contain one, two or four terms of the form

$$\mathrm{pqr} = \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky)\mathrm{r}(2\pi lz) \qquad \text{(A1.4.3.2)}$$

preceded by a signed numerical constant, where p, q and r can each be either a sine or a cosine function, and the arguments of the functions in any product of the form (A1.4.3.2) are ordered as in (A1.4.3.2). These products are given in this table as ccc, ccs, csc, scc, ssc, scs, css and/or sss, where c and s are abbreviations for 'sin' and 'cos', respectively.

Note that pqr vanishes if at least one of p, q and r is a sine, and the corresponding index *h*, *k* or *l* is zero.

No.	Symbol	Origin	Parity	*A*	*B*
16	$P222$			4ccc	−4sss
17	$P222_1$		$l = 2n$	4ccc	−4sss
			$l = 2n+1$	−4css	4scc
18	$P2_12_12$		$h+k = 2n$	4ccc	−4sss
			$h+k = 2n+1$	−4ssc	4ccs
19	$P2_12_12_1$		$h+k = 2n$; $k+l = 2n$	4ccc	−4sss
			$h+k = 2n$; $k+l = 2n+1$	−4css	4scc
			$h+k = 2n+1$; $k+l = 2n$	−4scs	4csc
			$h+k = 2n+1$; $k+l = 2n+1$	−4ssc	4ccs
20	$C222_1$		$l = 2n$	8ccc	−8sss
			$l = 2n+1$	−8css	8scc
21	$C222$			8ccc	−8sss
22	$F222$			16ccc	−16sss
23	$I222$			8ccc	−8sss
24	$I2_12_12_1$		h, k, l all even	8ccc	−8sss
			$h = 2n$; $k, l = 2n+1$	−8scs	8csc
			$k = 2n$; $l, h = 2n+1$	−8ssc	8ccs
			$l = 2n$; $h, k = 2n+1$	−8css	8scc
25	$Pmm2$			4ccc	4ccs
26	$Pmc2_1$		$l = 2n$	4ccc	4ccs
			$l = 2n+1$	−4css	4csc
27	$Pcc2$		$l = 2n$	4ccc	4ccs
			$l = 2n+1$	−4ssc	−4sss
28	$Pma2$		$h = 2n$	4ccc	4ccs
			$h = 2n+1$	−4ssc	−4sss
29	$Pca2_1$		$h = 2n$; $l = 2n$	4ccc	4ccs
			$h = 2n$; $l = 2n+1$	−4scs	4scc
			$h = 2n+1$; $l = 2n$	−4ssc	−4sss
			$h = 2n+1$; $l = 2n+1$	−4css	4csc
30	$Pnc2$		$k+l = 2n$	4ccc	4ccs
			$k+l = 2n+1$	−4ssc	4sss
31	$Pmn2_1$		$h+l = 2n$	4ccc	4ccs
			$h+l = 2n+1$	−4css	4csc
32	$Pba2$		$h+k = 2n$	4ccc	4ccs
			$h+k = 2n+1$	−4ssc	−4sss
33	$Pna2_1$		$h+k = 2n$; $l = 2n$	4ccc	4ccs
			$h+k = 2n$; $l = 2n+1$	−4scs	4scc
			$h+k = 2n+1$; $l = 2n$	−4ssc	−4sss
			$h+k = 2n+1$; $l = 2n+1$	−4css	4csc
34	$Pnn2$		$h+k+l = 2n$	4ccc	4ccs
			$h+k+l = 2n+1$	−4ssc	−4sss
35	$Cmm2$			8ccc	8ccs
36	$Cmc2_1$		$l = 2n$	8ccc	8ccs
			$l = 2n+1$	−8css	8csc
37	$Ccc2$		$l = 2n$	8ccc	8ccs
			$l = 2n+1$	−8ssc	−8sss
38	$Amm2$			8ccc	8ccs
39	$Abm2$		$k = 2n$	8ccc	8ccs
			$k = 2n+1$	−8ssc	−8sss
40	$Ama2$		$h = 2n$	8ccc	8ccs

Table A1.4.3.4. *Orthorhombic space groups* (*cont.*)

No.	Symbol	Origin	Parity	A	B
			$h = 2n + 1$	−8ssc	−8sss
41	*Aba*2		$h + k = 2n$	8ccc	8ccs
			$h + k = 2n + 1$	−8ssc	−8sss
42	*Fmm*2			16ccc	16ccs
43	*Fdd*2		$h + k + l = 4n$	16ccc	16ccs
			$h + k + l = 4n + 1$	8(ccc − ssc −ccs − sss)	8(ccs − sss + ccc +ssc)
			$h + k + l = 4n + 2$	−16ssc	−16sss
			$h + k + l = 4n + 3$	8(ccc − ssc + ccs + sss)	8(ccs − sss − ccc − ssc)
44	*Imm*2			8ccc	8ccs
45	*Iba*2		$l = 2n$	8ccc	8ccs
			$l = 2n + 1$	−8ssc	−8sss
46	*Iam*2		$h = 2n$	8ccc	8ccs
			$h = 2n + 1$	−8ssc	−8sss
47	*Pmmm*			8ccc	0
48	*Pnnn*	(1)	$h + k + l = 2n$	8ccc	0
			$h + k + l = 2n + 1$	0	−8sss
48	*Pnnn*	(2)	$h + k = 2n$; $k + l = 2n$	8ccc	0
			$h + k = 2n$; $k + l = 2n + 1$	−8ssc	0
			$h + k = 2n + 1$; $k + l = 2n$	−8css	0
			$h + k = 2n + 1$; $k + l = 2n + 1$	−8scs	0
49	*Pccm*		$l = 2n$	8ccc	0
			$l = 2n + 1$	−8ssc	0
50	*Pban*	(1)	$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	0	−8sss
50	*Pban*	(2)	$h = 2n$; $k = 2n$	8ccc	0
			$h = 2n$; $k = 2n + 1$	−8scs	0
			$h = 2n + 1$; $k = 2n$	−8css	0
			$h = 2n + 1$; $k = 2n + 1$	−8ssc	0
51	*Pmma*		$h = 2n$	8ccc	0
			$h = 2n + 1$	−8scs	0
52	*Pnna*		$h = 2n$; $k + l = 2n$	8ccc	0
			$h = 2n$; $k + l = 2n + 1$	−8ssc	0
			$h = 2n + 1$; $k + l = 2n$	−8css	0
			$h = 2n + 1$; $k + l = 2n + 1$	−8scs	0
53	*Pmna*		$h + l = 2n$	8ccc	0
			$h + l = 2n + 1$	−8css	0
54	*Pcca*		$h = 2n$; $l = 2n$	8ccc	0
			$h = 2n$; $l = 2n + 1$	−8ssc	0
			$h = 2n + 1$; $l = 2n$	−8scs	0
			$h = 2n + 1$; $l = 2n + 1$	−8css	0
55	*Pbam*		$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	−8ssc	0
56	*Pccn*		$h + k = 2n$; $h + l = 2n$	8ccc	0
			$h + k = 2n$; $h + l = 2n + 1$	−8ssc	0
			$h + k = 2n + 1$; $h + l = 2n$	−8css	0
			$h + k = 2n + 1$; $h + l = 2n + 1$	−8scs	0
57	*Pbcm*		$k = 2n$; $l = 2n$	8ccc	0
			$k = 2n$; $l = 2n + 1$	−8css	0
			$k = 2n + 1$; $l = 2n$	−8ssc	0
			$k = 2n + 1$; $l = 2n + 1$	−8scs	0
58	*Pnnm*		$h + k + l = 2n$	8ccc	0
			$h + k + l = 2n + 1$	−8ssc	0
59	*Pmmn*	(1)	$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	0	8ccs
59	*Pmmn*	(2)	$h = 2n$; $k = 2n$	8ccc	0
			$h = 2n$; $k = 2n + 1$	−8css	0

Table A1.4.3.4. *Orthorhombic space groups* (*cont.*)

No.	Symbol	Origin	Parity	*A*	*B*
			$h = 2n + 1;\ k = 2n$	−8scs	0
			$h = 2n + 1;\ k = 2n + 1$	−8ssc	0
60	*Pbcn*		$h + k = 2n;\ l = 2n$	8ccc	0
			$h + k = 2n;\ l = 2n + 1$	−8css	0
			$h + k = 2n + 1;\ l = 2n$	−8scs	0
			$h + k = 2n + 1;\ l = 2n + 1$	−8ssc	0
61	*Pbca*		$h + k = 2n;\ k + l = 2n$	8ccc	0
			$h + k = 2n;\ k + l = 2n + 1$	−8css	0
			$h + k = 2n + 1;\ k + l = 2n$	−8scs	0
			$h + k = 2n + 1;\ k + l = 2n + 1$	−8ssc	0
62	*Pnma*		$h + l = 2n;\ k = 2n$	8ccc	0
			$h + l = 2n;\ k = 2n + 1$	−8ssc	0
			$h + l = 2n + 1;\ k = 2n$	−8scs	0
			$h + l = 2n + 1;\ k = 2n + 1$	−8css	0
63	*Cmcm*		$l = 2n$	16ccc	0
			$l = 2n + 1$	−16css	0
64	*Cmca*		$k + l = 2n$	16ccc	0
			$k + l = 2n + 1$	−16css	0
65	*Cmmm*			16ccc	0
66	*Cccm*		$l = 2n$	16ccc	0
			$l = 2n + 1$	−16ssc	0
67	*Cmma*		$h = 2n$	16ccc	0
			$h = 2n + 1$	−16css	0
68	*Ccca*	(1)	$h + l = 2n$	16ccc	0
			$h + l = 2n + 1$	0	−16sss
68	*Ccca*	(2)	$k = 2n;\ l = 2n$	16ccc	0
			$k = 2n;\ l = 2n + 1$	−16ssc	0
			$k = 2n + 1;\ l = 2n$	−16scs	0
			$k = 2n + 1;\ l = 2n + 1$	−16css	0
69	*Fmmm*			32ccc	0
70	*Fddd*	(1)	$h + k + l = 4n$	32ccc	0
			$h + k + l = 4n + 1$	16(ccc − sss)	*A*
			$h + k + l = 4n + 2$	0	−32sss
			$h + k + l = 4n + 3$	16(ccc + sss)	−*A*
70	*Fddd*	(2)	$h + k = 4n;\ k + l = 4n;\ l + h = 4n$	32ccc	0
			$h + k = 4n;\ k + l = 4n + 2;$ $l + h = 4n + 2$	−32ssc	0
			$h + k = 4n + 2;\ k + l = 4n;$ $l + h = 4n + 2$	−32css	0
			$h + k = 4n + 2;\ k + l = 4n + 2;$ $l + h = 4n$	−32scs	0
			$h + k = 4n + 2;\ k + l = 4n + 2;$ $l + h = 4n + 2$	− 16(ccc + ssc + scs + css)	0
			$h + k = 4n + 2;\ k + l = 4n;\ l + h = 4n$	16(ccc + ssc − scs − css)	0
			$h + k = 4n;\ k + l = 4n + 2;\ l + h = 4n$	16(ccc − ssc − scs + css)	0
			$h + k = 4n;\ k + l = 4n;\ l + h = 4n + 2$	16(ccc − ssc + scs − css)	0
71	*Immm*			16ccc	0
72	*Ibam*		$l = 2n$	16ccc	0
			$l = 2n + 1$	−16ssc	0
73	*Ibca*		$h = 2n;\ k = 2n$	16ccc	0
			$h = 2n;\ k = 2n + 1$	−16scs	0
			$h = 2n + 1;\ k = 2n$	−16ssc	0
			$h = 2n + 1;\ k = 2n + 1$	−16css	0
74	*Imma*		$k = 2n$	16ccc	0
			$k = 2n + 1$	−16css	0

Table A1.4.3.5. *Tetragonal space groups*

The symbols appearing in this table are based on the factorization of the scalar product appearing in equations (1.4.2.19) and (1.4.2.20) into its plane-group and unique-axis components. The symbols are

$$\begin{aligned} \mathrm{P(pq)} &= \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) + \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kx)\\ \mathrm{M(pq)} &= \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) - \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kx), \end{aligned} \qquad \text{(A1.4.3.3)}$$

where p and q can each be a sine or a cosine.

Explicit trigonometric functions given in the table follow the convention

$$\mathrm{c}(u) = \cos(2\pi u) \quad \mathrm{s}(u) = \sin(2\pi u).$$

Conditions for vanishing symbols:

$$\begin{gathered} \mathrm{P(ss)} = \mathrm{M(ss)} = 0 \text{ if } h = 0 \text{ or } k = 0,\\ \mathrm{P(sc)} = \mathrm{M(sc)} = 0 \text{ if } h = 0,\\ \mathrm{P(cs)} = \mathrm{M(cs)} = 0 \text{ if } k = 0,\\ \mathrm{M(cc)} = \mathrm{M(ss)} = 0 \text{ if } h = k \text{ or } h = -k, \end{gathered}$$

and any explicit sine function vanishes if all the indices (h and k, or l) appearing in its argument are zero.

*P*4 [No. 75]

hkl	A	B
All	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$

$P4_1$ [No. 76] (enantiomorphous to $P4_3$ [No. 78])

l	A	B
$4n$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$
$4n+1$	$-2[\mathrm{s}(hx+ky)\mathrm{s}(lz) - \mathrm{s}(hy-kx)\mathrm{c}(lz)]$	$2[\mathrm{s}(hx+ky)\mathrm{c}(lz) + \mathrm{s}(hy-kx)\mathrm{s}(lz)]$
$4n+2$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$
$4n+3$	$-2[\mathrm{s}(hx+ky)\mathrm{s}(lz) + \mathrm{s}(hy-kx)\mathrm{c}(lz)]$	$2[\mathrm{s}(hx+ky)\mathrm{c}(lz) - \mathrm{s}(hy-kx)\mathrm{s}(lz)]$

$P4_2$ [No. 77]

l	A	B
$2n$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$
$2n+1$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$

$P4_3$ [No. 78] (enantiomorphous to $P4_1$ [No. 76])

l	A	B
$4n$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$2[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$
$4n+1$	$-2[\mathrm{s}(hx+ky)\mathrm{s}(lz) + \mathrm{s}(hy-kx)\mathrm{c}(lz)]$	$2[\mathrm{s}(hx+ky)\mathrm{c}(lz) - \mathrm{s}(hy-kx)\mathrm{s}(lz)]$
$4n+2$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$	$2[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$
$4n+3$	$-2[\mathrm{s}(hx+ky)\mathrm{s}(lz) - \mathrm{s}(hy-kx)\mathrm{c}(lz)]$	$2[\mathrm{s}(hx+ky)\mathrm{c}(lz) + \mathrm{s}(hy-kx)\mathrm{s}(lz)]$

*I*4 [No. 79]

hkl	A	B
All	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$

$I4_1$ [No. 80]

$2h+l$	A	B
$4n$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{s}(lz)$
$4n+1$	$4[\mathrm{c}(hx+ky)\mathrm{c}(lz) + \mathrm{c}(hy-kx)\mathrm{s}(lz)]$	$4[\mathrm{c}(hx+ky)\mathrm{s}(lz) - \mathrm{c}(hy-kx)\mathrm{c}(lz)]$
$4n+2$	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$
$4n+3$	$4[\mathrm{c}(hx+ky)\mathrm{c}(lz) - \mathrm{c}(hy-kx)\mathrm{s}(lz)]$	$4[\mathrm{c}(hx+ky)\mathrm{s}(lz) + \mathrm{c}(hy-kx)\mathrm{c}(lz)]$

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$P\bar{4}$ [No. 81]

hkl	*A*	*B*
All	2[P(cc) − M(ss)]c(*lz*)	2[M(cc) − P(ss)]s(*lz*)

$I\bar{4}$ [No. 82]

hkl	*A*	*B*
All	4[P(cc) − M(ss)]c(*lz*)	4[M(cc) − P(ss)]s(*lz*)

$P4/m$ [No. 83]

hkl	*A*	*B*
All	4[P(cc) − M(ss)]c(*lz*)	0

$P4_2/m$ [No. 84] ($B = 0$ for all h, k, l)

l	*A*
$2n$	4[P(cc) − M(ss)]c(*lz*)
$2n + 1$	4[M(cc) − P(ss)]c(*lz*)

$P4/n$ [No. 85, Origin 1]

$h + k$	*A*	*B*
$2n$	4[P(cc) − M(ss)]c(*lz*)	0
$2n + 1$	0	4[M(cc) − P(ss)]s(*lz*)

$P4/n$ [No. 85, Origin 2] ($B = 0$ for all h, k, l)

h	*k*	*A*
$2n$	$2n$	4[P(cc) − M(ss)]c(*lz*)
$2n$	$2n + 1$	−4[P(cs) + M(sc)]s(*lz*)
$2n + 1$	$2n$	−4[M(cs) + P(sc)]s(*lz*)
$2n + 1$	$2n + 1$	4[M(cc) − P(ss)]c(*lz*)

$P4_2/n$ [No. 86, Origin 1]

$h + k + l$	*A*	*B*
$2n$	4[P(cc) − M(ss)]c(*lz*)	0
$2n + 1$	0	4[M(cc) − P(ss)]s(*lz*)

$P4_2/n$ [No. 86, Origin 2] ($B = 0$ for all h, k, l)

$h + k$	$k + l$	$h + l$	*A*
$2n$	$2n$	$2n$	4[P(cc) − M(ss)]c(*lz*)
$2n$	$2n + 1$	$2n + 1$	4[M(cc) − P(ss)]c(*lz*)
$2n + 1$	$2n + 1$	$2n$	−4[M(cs) + P(sc)]s(*lz*)
$2n + 1$	$2n$	$2n + 1$	−4[P(cs) + M(sc)]s(*lz*)

$I4/m$ [No. 87]

hkl	*A*	*B*
All	8[P(cc) − M(ss)]c(*lz*)	0

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$I4_1/a$ [No. 88, Origin 1]

$2k+l$	A	B
$4n$	8[P(cc) − M(ss)]c(lz)	0
$4n+1$	4[P(cc) − M(ss)]c(lz) + [M(cc) − P(ss)]s(lz)	A
$4n+2$	0	8[M(cc) − P(ss)]s(lz)
$4n+3$	4[P(cc) − M(ss)]c(lz) − [M(cc) − P(ss)]s(lz)	$-A$

$I4_1/a$ [No. 88, Origin 2] ($B = 0$ for all h, k, l)

h	k	$h+k+l$	A
$2n$	$2n$	$4n$	8[P(cc) − M(ss)]c(lz)
$2n$	$2n+1$	$4n$	−8[s($hx+ky$)s(lz) − c($hy-kx$)c(lz)]
$2n+1$	$2n$	$4n$	8[c($hx+ky$)c(lz) − s($hy-kx$)s(lz)]
$2n+1$	$2n+1$	$4n$	−8[M(cs) + P(sc)]s(lz)
$2n$	$2n$	$4n+2$	8[M(cc) − P(ss)]c(lz)
$2n$	$2n+1$	$4n+2$	−8[s($hx+ky$)s(lz) + c($hy-kx$)c(lz)]
$2n+1$	$2n$	$4n+2$	8[c($hx+ky$)c(lz) + s($hy-kx$)s(lz)]
$2n+1$	$2n+1$	$4n+2$	−8[P(cs) + M(sc)]s(lz)

$P422$ [No. 89]

hkl	A	B
All	4P(cc)c(lz)	−4M(ss)s(lz)

$P42_12$ [No. 90]

$h+k$	A	B
$2n$	4P(cc)c(lz)	−4M(ss)s(lz)
$2n+1$	−4P(ss)c(lz)	4M(cc)s(lz)

$P4_122$ [No. 91] (enantiomorphous to $P4_322$ [No. 95])

l	A	B
$4n$	4P(cc)c(lz)	−4M(ss)s(lz)
$4n+1$	−4[s(hx)c(ky)s(lz) − c(kx)s(hy)c(lz)]	4[c(hx)s(ky)c(lz) − s(kx)c(hy)s(lz)]
$4n+2$	4M(cc)c(lz)	−4P(ss)s(lz)
$4n+3$	−4[s(hx)c(ky)s(lz) + c(kx)s(hy)c(lz)]	4[c(hx)s(ky)c(lz) + s(kx)c(hy)s(lz)]

$P4_12_12$ [No. 92] (enantiomorphous to $P4_32_12$ [No. 96])

$2h+2k+l$	A	B
$4n$	4P(cc)c(lz)	−4M(ss)s(lz)
$4n+1$	2{[P(sc) − P(cs)]c(lz) − [M(cs) − M(sc)]s(lz)}	2{[P(sc) + P(cs)]c(lz) + [M(cs) − M(sc)]s(lz)}
$4n+2$	−4P(ss)c(lz)	4M(cc)s(lz)
$4n+3$	−2{[P(sc) − P(cs)]c(lz) + [M(cs) + M(sc)]s(lz)}	2{[P(sc) + P(cs)]c(lz) − [M(cs) − M(sc)s(lz)}

$P4_222$ [No. 93]

l	A	B
$2n$	4P(cc)c(lz)	−4M(ss)s(lz)
$2n+1$	4M(cc)c(lz)	−4P(ss)s(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$P4_22_12$ [No. 94]

$h+k+l$	A	B
$2n$	4P(cc)c(lz)	−4M(ss)s(lz)
$2n+1$	−4P(ss)c(lz)	4M(cc)s(lz)

$P4_322$ [No. 95] (enantiomorphous to $P4_122$ [No. 91])

l	A	B
$4n$	4P(cc)c(lz)	−4M(ss)s(lz)
$4n+1$	−4[s(hx)c(ky)s(lz) + c(kx)s(hy)c(lz)]	4[c(hx)s(ky)c(lz) + s(kx)c(hy)c(lz)]
$4n+2$	4M(cc)c(lz)	−4P(ss)s(lz)
$4n+3$	−4[s(hx)c(ky)s(lz) − c(kx)s(hy)c(lz)]	4[c(hx)s(ky)c(lz) − s(kx)c(hy)c(lz)]

$P4_32_12$ [No. 96] (enantiomorphous to $P4_12_12$ [No. 92])

$2h+2k+l$	A	B
$4n$	4P(cc)c(lz)	−4M(ss)s(lz)
$4n+1$	−2{[P(sc) − P(cs)]c(lz) + [M(cs) + M(sc)]s(lz)}	2{[P(sc) + P(cs)]c(lz) − [M(cs) − M(sc)]s(lz)}
$4n+2$	−4P(ss)c(lz)	4M(cc)s(lz)
$4n+3$	2{[P(sc) − P(cs)]c(lz) − [M(cs) + M(sc)]s(lz)}	2{[P(sc) + P(cs)]c(lz) + [M(cs) − M(sc)]s(lz)}

$I422$ [No. 97]

hkl	A	B
All	8P(cc)c(lz)	−8M(ss)s(lz)

$I4_122$ [No. 98]

$2k+l$	A	B
$4n$	8P(cc)c(lz)	−8M(ss)s(lz)
$4n+1$	4{[P(cc) − P(ss)]c(lz) + [M(cc) + M(ss)]s(lz)}	4{[P(cc) + P(ss)]c(lz) + [M(cc) − M(ss)]s(lz)}
$4n+2$	−8P(ss)c(lz)	8M(cc)s(lz)
$4n+3$	4{[P(cc) − P(ss)]c(lz) − [M(cc) + M(ss)]s(lz)}	−4{[P(cc) + P(ss)]c(lz) − [M(cc) − M(ss)]s(lz)}

$P4mm$ [No. 99]

hkl	A	B
All	4P(cc)c(lz)	4P(cc)s(lz)

$P4bm$ [No. 100]

$h+k$	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4M(ss)s(lz)

$P4_2cm$ [No. 101]

l	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	−4P(ss)c(lz)	−4P(ss)s(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$P4_2nm$ [No. 102]

$h+k+l$	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	−4P(ss)c(lz)	−4P(ss)s(lz)

$P4cc$ [No. 103]

l	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4M(ss)s(lz)

$P4nc$ [No. 104]

$h+k+l$	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4M(ss)s(lz)

$P4_2mc$ [No. 105]

l	A	B
$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	4M(cc)c(lz)	4M(cc)s(lz)

$P4_2bc$ [No. 106]

$h+k$	l	A	B
$2n$	$2n$	4P(cc)c(lz)	4P(cc)s(lz)
$2n+1$	$2n$	−4M(ss)c(lz)	−4M(ss)s(lz)
$2n$	$2n+1$	4M(cc)c(lz)	4M(cc)s(lz)
$2n+1$	$2n+1$	−4P(ss)c(lz)	−4P(ss)s(lz)

$I4mm$ [No. 107]

hkl	A	B
All	8P(cc)c(lz)	8P(cc)s(lz)

$I4cm$ [No. 108]

l	A	B
$2n$	8P(cc)c(lz)	8P(cc)s(lz)
$2n+1$	−8M(ss)c(lz)	−8M(ss)s(lz)

$I4_1md$ [No. 109]

$2k+l$	A	B
$4n$	8P(cc)c(lz)	8P(cc)s(lz)
$4n+1$	8[c(hx)c(ky)c(lz) − c(kx)c(hy)s(lz)]	8[c(hx)c(ky)s(lz) + c(kx)c(hy)c(lz)]
$4n+2$	8M(cc)c(lz)	8M(cc)s(lz)
$4n+3$	8[c(hx)c(ky)c(lz) + c(kx)c(hy)s(lz)]	8[c(hx)c(ky)s(lz) − c(kx)c(hy)c(lz)]

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$I4_1cd$ [No. 110]

$2k+l$	A	B
$4n$	8P(cc)c(lz)	8P(cc)s(lz)
$4n+1$	−8[s(hx)s(ky)c(lz) + s(kx)s(hy)s(lz)]	−8[s(hx)s(ky)s(lz) − s(kx)s(hy)c(lz)]
$4n+2$	8M(cc)c(lz)	8M(cc)s(lz)
$4n+3$	−8[s(hx)s(ky)c(lz) − s(kx)s(hy)s(lz)]	−8[s(hx)s(ky)s(lz) + s(kx)s(hy)c(lz)]

$P\bar{4}2m$ [No. 111]

hkl	A	B
All	4P(cc)c(lz)	−4P(ss)s(lz)

$P\bar{4}2c$ [No. 112]

l	A	B
$2n$	4P(cc)c(lz)	−4P(ss)s(lz)
$2n+1$	−4M(ss)c(lz)	4M(cc)s(lz)

$P\bar{4}2_1m$ [No. 113]

$h+k$	A	B
$2n$	4P(cc)c(lz)	−4P(ss)s(lz)
$2n+1$	−4M(ss)c(lz)	4M(cc)s(lz)

$P\bar{4}2_1c$ [No. 114]

$h+k+l$	A	B
$2n$	4P(cc)c(lz)	−4P(ss)s(lz)
$2n+1$	−4M(ss)c(lz)	4M(cc)s(lz)

$P\bar{4}m2$ [No. 115]

hkl	A	B
All	4P(cc)c(lz)	4M(cc)s(lz)

$P\bar{4}c2$ [No. 116]

l	A	B
$2n$	4P(cc)c(lz)	4M(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4P(ss)s(lz)

$P\bar{4}b2$ [No. 117]

$h+k$	A	B
$2n$	4P(cc)c(lz)	4M(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4P(ss)s(lz)

$P\bar{4}n2$ [No. 118]

$h+k+l$	A	B
$2n$	4P(cc)c(lz)	4M(cc)s(lz)
$2n+1$	−4M(ss)c(lz)	−4P(ss)s(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$I\bar{4}m2$ [No. 119]

hkl	A	B
All	8P(cc)c(lz)	8M(cc)s(lz)

$I\bar{4}c2$ [No. 120]

l	A	B
$2n$	8P(cc)c(lz)	8M(cc)s(lz)
$2n+1$	−8M(ss)c(lz)	−8P(ss)s(lz)

$I\bar{4}2m$ [No. 121]

hkl	A	B
All	8P(cc)c(lz)	−8P(ss)s(lz)

$I\bar{4}2d$ [No. 122]

$2h+l$	A	B
$4n$	8P(cc)c(lz)	−8P(ss)s(lz)
$4n+1$	4{[P(cc) − M(ss)]c(lz) − [M(cc) + P(ss)]s(lz)}	−4{[P(cc) + M(ss)]c(lz) − [M(cc) − P(ss)]s(lz)}
$4n+2$	−8M(ss)c(lz)	8M(cc)s(lz)
$4n+3$	4{[P(cc) − M(ss)]c(lz) + [M(cc) + P(ss)]s(lz)}	4{[P(cc) + M(ss)]c(lz) + [M(cc) − P(ss)]s(lz)}

$P4/mmm$ [No. 123]

hkl	A	B
All	8P(cc)c(lz)	0

$P4/mcc$ [No. 124] ($B = 0$ for all h, k, l)

l	A
$2n$	8P(cc)c(lz)
$2n+1$	−8M(ss)c(lz)

$P4/nbm$ [No. 125, Origin 1]

$h+k$	A	B
$2n$	8P(cc)c(lz)	0
$2n+1$	0	−8M(ss)s(lz)

$P4/nbm$ [No. 125, Origin 2] ($B = 0$ for all h, k, l)

h	k	A
$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n+1$	−8M(sc)s(lz)
$2n+1$	$2n$	−8M(cs)s(lz)
$2n+1$	$2n+1$	−8P(ss)c(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

*P*4/*nnc* [No. 126, Origin 1]

$h+k+l$	*A*	*B*
$2n$	8P(cc)c(lz)	0
$2n+1$	0	−8M(ss)s(lz)

*P*4/*nnc* [No. 126, Origin 2] ($B = 0$ for all h, k, l)

h	*k*	*l*	*A*
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n$	$2n+1$	−8M(ss)c(lz)
$2n$	$2n+1$	$2n$	−8M(sc)s(lz)
$2n$	$2n+1$	$2n+1$	−8P(cs)s(lz)
$2n+1$	$2n$	$2n$	−8M(cs)s(lz)
$2n+1$	$2n$	$2n+1$	−8P(sc)s(lz)
$2n+1$	$2n+1$	$2n$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n+1$	8M(cc)c(lz)

*P*4/*mbm* [No. 127] ($B = 0$ for all h, k, l)

$h+k$	*A*
$2n$	8P(cc)c(lz)
$2n+1$	−8M(ss)c(lz)

*P*4/*mnc* [No. 128] ($B = 0$ for all h, k, l)

$h+k+l$	*A*
$2n$	8P(cc)c(lz)
$2n+1$	−8M(ss)c(lz)

*P*4/*nmm* [No. 129, Origin 1]

$h+k$	*A*	*B*
$2n$	8P(cc)c(lz)	0
$2n+1$	0	8M(cc)s(lz)

*P*4/*nmm* [No. 129, Origin 2] ($B = 0$ for all h, k, l)

h	*k*	*A*
$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n+1$	−8P(cs)s(lz)
$2n+1$	$2n$	−8P(sc)s(lz)
$2n+1$	$2n+1$	−8P(ss)c(lz)

*P*4/*ncc* [No. 130, Origin 1]

$h+k$	*l*	*A*	*B*
$2n$	$2n$	8P(cc)c(lz)	0
$2n$	$2n+1$	−8M(ss)c(lz)	0
$2n+1$	$2n$	0	8M(cc)s(lz)
$2n+1$	$2n+1$	0	−8P(ss)s(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

*P*4/*ncc* [No. 130, Origin 2] ($B = 0$ for all h, k, l)

h	k	l	A
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n$	$2n+1$	−8M(ss)c(lz)
$2n$	$2n+1$	$2n$	−8P(cs)s(lz)
$2n$	$2n+1$	$2n+1$	−8M(sc)s(lz)
$2n+1$	$2n$	$2n$	−8P(sc)s(lz)
$2n+1$	$2n$	$2n+1$	−8M(cs)s(lz)
$2n+1$	$2n+1$	$2n$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n+1$	8M(cc)c(lz)

$P4_2/mmc$ [No. 131] ($B = 0$ for all h, k, l)

l	A
$2n$	8P(cc)c(lz)
$2n+1$	8M(cc)c(lz)

$P4_2/mcm$ [No. 132] ($B = 0$ for all h, k, l)

l	A
$2n$	8P(cc)c(lz)
$2n+1$	−8P(ss)c(lz)

$P4_2/nbc$ [No. 133, Origin 1]

$h+k+l$	l	A	B
$2n$	$2n$	8P(cc)c(lz)	0
$2n$	$2n+1$	−8M(ss)c(lz)	0
$2n+1$	$2n$	0	−8P(ss)s(lz)
$2n+1$	$2n+1$	0	8M(cc)s(lz)

$P4_2/nbc$ [No. 133, Origin 2] ($B = 0$ for all h, k, l)

h	k	l	A
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n$	$2n+1$	8M(cc)c(lz)
$2n$	$2n+1$	$2n$	−8M(sc)s(lz)
$2n$	$2n+1$	$2n+1$	−8P(sc)s(lz)
$2n+1$	$2n$	$2n$	−8M(cs)s(lz)
$2n+1$	$2n$	$2n+1$	−8P(cs)s(lz)
$2n+1$	$2n+1$	$2n$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n+1$	−8M(ss)c(lz)

$P4_2/nnm$ [No. 134, Origin 1]

$h+k+l$	A	B
$2n$	8P(cc)c(lz)	0
$2n+1$	0	−8P(ss)s(lz)

$P4_2/nnm$ [No. 134, Origin 2] ($B = 0$ for all h, k, l)

$h+k$	$k+l$	$h+l$	A
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n+1$	$2n+1$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n$	−8M(sc)s(lz)
$2n+1$	$2n$	$2n+1$	−8M(cs)s(lz)

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$P4_2/mbc$ [No. 135] ($B = 0$ for all h, k, l)

$h+k$	l	A
$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n+1$	8M(cc)c(lz)
$2n+1$	$2n$	−8M(ss)c(lz)
$2n+1$	$2n+1$	−8P(ss)c(lz)

$P4_2/mnm$ [No. 136] ($B = 0$ for all h, k, l)

$h+k+l$	A
$2n$	8P(cc)c(lz)
$2n+1$	−8P(ss)c(lz)

$P4_2/nmc$ [No. 137, Origin 1]

$h+k+l$	A	B
$2n$	8P(cc)c(lz)	0
$2n+1$	0	8M(cc)s(lz)

$P4_2/nmc$ [No. 137, Origin 2] ($B = 0$ for all h, k, l)

h	k	l	A
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n$	$2n+1$	8M(cc)c(lz)
$2n$	$2n+1$	$2n$	−8P(cs)s(lz)
$2n$	$2n+1$	$2n+1$	−8M(cs)s(lz)
$2n+1$	$2n$	$2n$	−8P(sc)s(lz)
$2n+1$	$2n$	$2n+1$	−8M(sc)s(lz)
$2n+1$	$2n+1$	$2n$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n+1$	−8M(ss)c(lz)

$P4_2/ncm$ [No. 138, Origin 1]

$h+k$	l	A	B
$2n$	$2n$	8P(cc)c(lz)	0
$2n+1$	$2n+1$	−8M(ss)c(lz)	0
$2n+1$	$2n$	0	8M(cc)s(lz)
$2n$	$2n+1$	0	−8P(ss)s(lz)

$P4_2/ncm$ [No. 138, Origin 2] ($B = 0$ for all h, k, l)

$h+k$	$k+l$	$h+l$	A
$2n$	$2n$	$2n$	8P(cc)c(lz)
$2n$	$2n+1$	$2n+1$	−8P(ss)c(lz)
$2n+1$	$2n+1$	$2n$	−8P(cs)s(lz)
$2n+1$	$2n$	$2n+1$	−8P(sc)s(lz)

$I4/mmm$ [No. 139]

hkl	A	B
All	16P(cc)c(lz)	0

Table A1.4.3.5. *Tetragonal space groups* (*cont.*)

$I4/mcm$ [No. 140] ($B = 0$ for all h, k, l)

l	A
$2n$	16P(cc)c(lz)
$2n + 1$	−16M(ss)c(lz)

$I4_1/amd$ [No. 141, Origin 1]

$2h + l$	A	B
$4n$	16P(cc)c(lz)	0
$4n + 1$	8[P(cc)c(lz) − M(cc)s(lz)]	$-A$
$4n + 2$	0	16M(cc)s(lz)
$4n + 3$	8[P(cc)c(lz) + M(cc)s(lz)]	A

$I4_1/amd$ [No. 141, Origin 2] ($B = 0$ for all h, k, l)

h	k	$h + k + l$	A
$2n$	$2n$	$4n$	16P(cc)c(lz)
$2n$	$2n + 1$	$4n$	−16[c(hx)s(ky)s(lz) + c(kx)c(hy)c(lz)]
$2n + 1$	$2n$	$4n$	16[c(hx)c(ky)c(lz) + c(kx)s(hy)s(lz)]
$2n + 1$	$2n + 1$	$4n$	−16[c(hx)s(ky)s(lz) + c(kx)s(hy)s(lz)]
$2n$	$2n$	$4n + 2$	16M(cc)c(lz)
$2n$	$2n + 1$	$4n + 2$	−16[c(hx)s(ky)s(lz) − c(kx)c(hy)c(lz)]
$2n + 1$	$2n$	$4n + 2$	16[c(hx)c(ky)c(lz) − c(kx)s(hy)s(lz)]
$2n + 1$	$2n + 1$	$4n + 2$	−16[c(hx)s(ky)s(lz) − c(kx)s(hy)s(lz)]

$I4_1/acd$ [No. 142, Origin 1]

$2h + l$	A	B
$4n$	16P(cc)c(lz)	0
$4n + 1$	−8[M(ss)c(lz) − P(ss)s(lz)]	$-A$
$4n + 2$	0	16M(cc)s(lz)
$4n + 3$	−8[M(ss)c(lz) + P(ss)s(lz)]	A

$I4_1/acd$ [No. 142, Origin 2] ($B = 0$ for all h, k, l)

h	k	$h + k + l$	A
$2n$	$2n$	$4n$	16P(cc)c(lz)
$2n$	$2n + 1$	$4n$	−16[s(hx)c(ky)s(lz) + s(kx)s(hy)c(lz)]
$2n + 1$	$2n$	$4n$	−16[s(hx)s(ky)c(lz) + s(kx)c(hy)s(lz)]
$2n + 1$	$2n + 1$	$4n$	−16[c(hx)s(ky)s(lz) + c(kx)s(hy)s(lz)]
$2n$	$2n$	$4n + 2$	16M(cc)c(lz)
$2n$	$2n + 1$	$4n + 2$	−16[s(hx)c(ky)s(lz) − s(kx)s(hy)c(lz)]
$2n + 1$	$2n$	$4n + 2$	−16[s(hx)s(ky)c(lz) − s(kx)c(hy)s(lz)]
$2n + 1$	$2n + 1$	$4n + 2$	−16[c(hx)s(ky)s(lz) − c(kx)s(hy)s(lz)]

Table A1.4.3.6. *Trigonal and hexagonal space groups*

The table lists the expressions for A and B for the space groups belonging to the hexagonal family. For the space groups that are referred to hexagonal axes the expressions are given in terms of symbols related to the decomposition of the scalar products into their plane-group and unique-axis components [*cf.* equations (1.4.3.10)–(1.4.3.12)]. The symbols for the seven rhombohedral space groups in their rhombohedral-axes representation are the same as those used for the cubic space groups [*cf.* equations (1.4.3.4) and (1.4.3.5), and the notes at the start of Table A1.4.3.7]. Factors of the forms $\cos(2\pi x)$ and $\sin(2\pi x)$ are abbreviated by $c(x)$ and $s(x)$, respectively. All the symbols used in this table are repeated below. Most expressions are given in terms of

$$\begin{aligned} C(hki) &= c(p_1) + c(p_2) + c(p_3), \\ C(khi) &= c(q_1) + c(q_2) + c(q_3) \text{ and} \\ S(hki) &= s(p_1) + s(p_2) + s(p_3), \\ S(khi) &= s(q_1) + s(q_2) + s(q_3), \end{aligned} \quad \text{(A1.4.3.4)}$$

where

$$\begin{aligned} p_1 &= hx + ky, \quad p_2 = kx + iy, \quad p_3 = ix + hy, \\ q_1 &= kx + hy, \quad q_2 = hx + iy, \quad q_3 = ix + ky, \end{aligned} \quad \text{(A1.4.3.5)}$$

and the abbreviations

$$\begin{aligned} PH(cc) &= C(hki) + C(khi), \\ PH(ss) &= S(hki) + S(khi), \\ MH(cc) &= C(hki) - C(khi) \text{ and} \\ MH(ss) &= S(hki) - S(khi). \end{aligned} \quad \text{(A1.4.3.6)}$$

In addition, the following abbreviations are employed for some space groups:

$$u_1 = lz, \quad u_2 = lz + \tfrac{1}{3} \text{ and } u_3 = lz - \tfrac{1}{3}.$$

Conditons for vanishing symbols:

$$\begin{aligned} S(hki) = S(khi) = 0 &\text{ if } h = k = 0, \\ PH(ss) = 0 &\text{ if } h = -k \text{ (or } k = -i \text{ or } i = -h), \\ MH(cc) = 0 &\text{ if } |h| = |k| \text{ (or } |k| = |i| \text{ or } |i| = |h|) \end{aligned}$$

and any explicit sine function vanishes if all the indices (h and k, or l) appearing in its argument are zero.

*P*3 [No. 143]

hkl	*A*	*B*
All	$C(hki)c(lz) - S(hki)s(lz)$	$C(hki)s(lz) + S(hki)c(lz)$

$P3_1$ [No. 144] (enantiomorphous to $P3_2$ [No. 145])

l	*A*	*B*
$3n$	as for *P*3 [No. 143]	
$3n+1$	$c(p_1+u_1) + c(p_2+u_2) + c(p_3+u_3)$	$s(p_1+u_1) + s(p_2+u_2) + s(p_3+u_3)$
$3n+2$	$c(p_1+u_1) + c(p_2+u_3) + c(p_3+u_2)$	$s(p_1+u_1) + s(p_2+u_3) + s(p_3+u_2)$

$P3_2$ [No. 145] (enantiomorphous to $P3_1$ [No. 144])

l	*A*, *B*
$3n$	as for *P*3 [No. 143]
$3n+1$	as for $l = 3n+2$ in $P3_1$ [No. 144]
$3n+2$	as for $l = 3n+1$ in $P3_1$ [No. 144]

*R*3 [No. 146] (rhombohedral axes)

hkl	*A*	*B*
All	$c(hx+ky+lz) + c(kx+ly+hz) + c(lx+hy+kz)$	$s(hx+ky+lz) + s(kx+ly+hz) + s(lx+hy+kz)$

*R*3 [No. 146] (hexagonal axes)

hkl	*A*	*B*
All	$3[C(hki)c(lz) - S(hki)s(lz)]$	$3[C(hki)s(lz) + S(hki)c(lz)]$

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

$P\bar{3}$ [No. 147]

hkl	A	B
All	$2[C(hki)c(lz) - S(hki)s(lz)]$	0

$R\bar{3}$ [No. 148] (rhombohedral axes)

hkl	A	B
All	$2[c(hx+ky+lz) + c(kx+ly+hz) + c(lx+hy+kz)]$	0

$R\bar{3}$ [No. 148] (hexagonal axes)

hkl	A	B
All	$6[C(hki)c(lz) - S(hki)s(lz)]$	0

$P312$ [No. 149]

hkl	A	B
All	$PH(cc)c(lz) - PH(ss)s(lz)$	$MH(cc)s(lz) + MH(ss)c(lz)$

$P321$ [No. 150]

hkl	A	B
All	$PH(cc)c(lz) - MH(ss)s(lz)$	$PH(ss)c(lz) + MH(cc)s(lz)$

$P3_112$ [No. 151] (enantiomorphous to $P3_212$ [No. 153])

l	A	B
$3n$	as for $P312$ [No. 149]	
$3n+1$	$c(p_1+u_1)+c(p_2+u_2)+c(p_3+u_3)+c(q_1+u_2)$ $+ c(q_2+u_3)+c(q_3+u_1)]$	$s(p_1+u_1)+s(p_2+u_2)+s(p_3+u_3)-s(q_1+u_2)$ $- s(q_2+u_3)-s(q_3+u_1)$
$3n+2$	$c(p_1+u_1)+c(p_2+u_3)+c(p_3+u_2)+c(q_1+u_3)$ $+ c(q_2+u_2)+c(q_3+u_1)$	$s(p_1+u_1)+s(p_2+u_3)+s(p_3+u_2)-s(q_1+u_3)$ $- s(q_2+u_2)-s(q_3+u_1)$

$P3_121$ [No. 152] (enantiomorphous to $P3_221$ [No. 154])

l	A	B
$3n$	as for $P321$ [No. 150]	
$3n+1$	$c(p_1+u_1)+c(p_2+u_2)+c(p_3+u_3)+c(q_1-u_1)$ $+ c(q_2-u_2)+c(q_3-u_3)$	$s(p_1+u_1)+s(p_2+u_2)+s(p_3+u_3)+s(q_1-u_1)$ $+ s(q_2-u_2)+s(q_3-u_3)$
$3n+2$	$c(p_1+u_1)+c(p_2+u_3)+c(p_3+u_2)+c(q_1-u_1)$ $+ c(q_2-u_3)+c(q_3-u_2)$	$s(p_1+u_1)+s(p_2+u_3)+s(p_3+u_2)+s(q_1-u_1)$ $+ s(q_2-u_3)+s(q_3-u_2)$

$P3_212$ [No. 153] (enantiomorphous to $P3_112$ [No. 151])

l	A, B
$3n$	as for $P312$ [No. 149]
$3n+1$	as for $l = 3n+2$ in $P3_112$ [No. 151]
$3n+2$	as for $l = 3n+1$ in $P3_112$ [No. 151]

$P3_221$ [No. 154] (enantiomorphous to $P3_121$ [No. 152])

l	A, B
$3n$	as for $P321$ [No. 150]
$3n+1$	as for $l = 3n+2$ in $P3_121$ [No. 152]
$3n+2$	as for $l = 3n+1$ in $P3_121$ [No. 152]

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

*R*32 [No. 155] (rhombohedral axes)

hkl	*A*	*B*
All	Eccc − Ecss − Escs − Essc + Occc − Ocss − Oscs − Ossc	Escc + Ecsc + Eccs − Esss − Oscc − Ocsc − Occs + Osss

*R*32 [No. 155] (hexagonal axes)

hkl	*A*	*B*
All	3[PH(cc)c(*lz*) − MH(ss)s(*lz*)]	3[PH(ss)c(*lz*) + MH(cc)s(*lz*)]

*P*3*m*1 [No. 156]

hkl	*A*	*B*
All	PH(cc)c(*lz*) − MH(ss)s(*lz*)	PH(cc)s(*lz*) + MH(ss)c(*lz*)

*P*31*m* [No. 157]

hkl	*A*	*B*
All	PH(cc)c(*lz*) − PH(ss)s(*lz*)	PH(cc)s(*lz*) + PH(ss)c(*lz*)

*P*3*c*1 [No. 158]

l	*A*	*B*
2*n*	PH(cc)c(*lz*) − MH(ss)s(*lz*)	PH(cc)s(*lz*) + MH(ss)c(*lz*)
2*n* + 1	MH(cc)c(*lz*) − PH(ss)s(*lz*)	PH(ss)c(*lz*) + MH(cc)s(*lz*)

*P*31*c* [No. 159]

l	*A*	*B*
2*n*	PH(cc)c(*lz*) − PH(ss)s(*lz*)	PH(cc)s(*lz*) + PH(ss)c(*lz*)
2*n* + 1	MH(cc)c(*lz*) − MH(ss)s(*lz*)	MH(cc)s(*lz*) + MH(ss)c(*lz*)

*R*3*m* [No. 160] (rhombohedral axes)

hkl	*A*	*B*
All	Eccc − Ecss − Escs − Essc + Occc − Ocss − Oscs − Ossc	Escc + Ecsc + Eccs − Esss + Oscc + Ocsc + Occs − Osss

*R*3*m* [No. 160] (hexagonal axes)

hkl	*A*	*B*
All	3[PH(cc)c(*lz*) − MH(ss)s(*lz*)]	3[PH(cc)s(*lz*) + MH(ss)c(*lz*)]

*R*3*c* [No. 161] (rhombohedral axes)

$h+k+l$	*A*	*B*
2*n*	Eccc − Ecss − Escs − Essc + Occc − Ocss − Oscs − Ossc	Escc + Ecsc + Eccs − Esss + Oscc + Ocsc + Occs − Osss
2*n* + 1	Eccc − Ecss − Escs − Essc − Occc + Ocss + Oscs + Ossc	Escc + Ecsc + Eccs − Esss − Oscc − Ocsc − Occs + Osss

*R*3*c* [No. 161] (hexagonal axes)

l	*A*	*B*
2*n*	3[PH(cc)c(*lz*) − MH(ss)s(*lz*)]	3[PH(cc)s(*lz*) + MH(ss)c(*lz*)]
2*n* + 1	3[MH(cc)c(*lz*) − PH(ss)s(*lz*)]	3[PH(ss)c(*lz*) + MH(cc)s(*lz*)]

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

$P\bar{3}1m$ [No. 162] ($B = 0$ for all h, k, l)

A
2[PH(cc)c(lz) − PH(ss)s(lz)]

$P\bar{3}1c$ [No. 163] ($B = 0$ for all h, k, l)

l	A
$2n$	2[PH(cc)c(lz) − PH(ss)s(lz)]
$2n + 1$	2[MH(cc)c(lz) − MH(ss)s(lz)]

$P\bar{3}m1$ [No. 164] ($B = 0$ for all h, k, l)

A
2[PH(cc)c(lz) − MH(ss)s(lz)]

$P\bar{3}c1$ [No. 165] ($B = 0$ for all h, k, l)

l	A
$2n$	2[PH(cc)c(lz) − MH(ss)s(lz)]
$2n + 1$	2[MH(cc)c(lz) − PH(ss)s(lz)]

$R\bar{3}m$ [No. 166] (rhombohedral axes, $B = 0$ for all h, k, l)

A
2(Eccc − Ecss − Escs − Essc + Occc − Ocss − Oscs − Ossc)

$R\bar{3}m$ [No. 166] (hexagonal axes, $B = 0$ for all h, k, l)

A
6[PH(cc)c(lz) − MH(ss)s(lz)]

$R\bar{3}c$ [No. 167] (rhombohedral axes, $B = 0$ for all h, k, l)

$h + k + l$	A
$2n$	2(Eccc − Ecss − Escs − Essc + Occc − Ocss − Oscs − Ossc)
$2n + 1$	2(Eccc − Ecss − Escs − Essc − Occc + Ocss + Oscs + Ossc)

$R\bar{3}c$ [No. 167] (hexagonal axes, $B = 0$ for all h, k, l)

l	A
$2n$	6[PH(cc)c(lz) − MH(ss)s(lz)]
$2n + 1$	6[MH(cc)c(lz) − PH(ss)s(lz)]

$P6$ [No. 168]

hkl	A	B
All	2C(hki)c(lz)	2C(hki)s(lz)

$P6_1$ [No. 169] (enantiomorphous to $P6_5$ [No. 170])

l	A	B
$6n$	as for $P6$ [No.168]	
$6n + 1$	$-2[s(p_1)s(u_1) + s(p_2)s(u_2) + s(p_3)s(u_3)]$	$2[s(p_1)c(u_1) + s(p_2)c(u_2) + s(p_3)c(u_3)]$
$6n + 2$	$2[c(p_1)c(u_1) + c(p_2)c(u_3) + c(p_3)c(u_2)]$	$2[c(p_1)s(u_1) + c(p_2)s(u_3) + c(p_3)s(u_2)]$
$6n + 3$	−2S(hki)s(lz)	2S(hki)c(lz)
$6n + 4$	$2[c(p_1)c(u_1) + c(p_2)c(u_2) + c(p_3)c(u_3)]$	$2[c(p_1)s(u_1) + c(p_2)s(u_2) + c(p_3)s(u_3)]$
$6n + 5$	$-2[s(p_1)s(u_1) + s(p_2)s(u_3) + s(p_3)s(u_2)]$	$2[s(p_1)c(u_1) + s(p_2)c(u_3) + s(p_3)c(u_2)]$

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

$P6_5$ [No. 170] (enantiomorphous to $P6_1$ [No. 169])

l	A, B
$6n$	as for $P6$ [No. 168]
$6n+1$	as for $l = 6n+5$ in $P6_1$ [No. 169]
$6n+2$	as for $l = 6n+4$ in $P6_1$ [No. 169]
$6n+3$	as for $l = 6n+3$ in $P6_1$ [No. 169]
$6n+4$	as for $l = 6n+2$ in $P6_1$ [No. 169]
$6n+5$	as for $l = 6n+1$ in $P6_1$ [No. 169]

$P6_2$ [No. 171] (enantiomorphous to $P6_4$ [No. 172])

l	A, B
$3n$	as for $P6$ [No. 168]
$3n+1$	as for $l = 6n+2$ in $P6_1$ [No. 169]
$3n+2$	as for $l = 6n+4$ in $P6_1$ [No. 169]

$P6_4$ [No. 172] (enantiomorphous to $P6_2$ [No. 171])

l	A, B
$3n$	as for $P6$ [No. 168]
$3n+1$	as for $l = 6n+4$ in $P6_1$ [No.169]
$3n+2$	as for $l = 6n+2$ in $P6_1$ [No. 169]

$P6_3$ [No. 173]

l	A, B
$2n$	as for $P6$ [No. 168]
$2n+1$	as for $l = 6n+3$ in $P6_1$ [No. 169]

$P\bar{6}$ [No. 174]

hkl	A	B
All	2C(hki)c(lz)	2S(hki)c(lz)

$P6/m$ [No. 175]

hkl	A	B
All	4C(hki)c(lz)	0

$P6_3/m$ [No. 176]

l	A	B
$2n$	4C(hki)c(lz)	0
$2n+1$	−4S(hki)s(lz)	0

$P622$ [No. 177]

hkl	A	B
All	2PH(cc)c(lz)	2MH(cc)s(lz)

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

$P6_122$ [No. 178] (enantiomorphous to $P6_522$ [No. 179])

l	A	B
$6n$	as for $P622$ [No. 177]	
$6n+1$	$-2[s(p_1)s(u_1)+s(p_2)s(u_2)+s(p_3)s(u_3)-s(q_1)s(u_3)$ $-s(q_2)s(u_1)-s(q_3)s(u_2)]$	$2[s(p_1)c(u_1)+s(p_2)c(u_2)+s(p_3)c(u_3)+s(q_1)c(u_3)$ $+s(q_2)c(u_1)+s(q_3)c(u_2)]$
$6n+2$	$2[c(p_1)c(u_1)+c(p_2)c(u_3)+c(p_3)c(u_2)+c(q_1)c(u_2)$ $+c(q_2)c(u_1)+c(q_3)c(u_3)]$	$2[c(p_1)s(u_1)+c(p_2)s(u_3)+c(p_3)s(u_2)-c(q_1)s(u_2)$ $-c(q_2)s(u_1)-c(q_3)s(u_3)]$
$6n+3$	$-2\mathrm{MH(ss)s}(lz)$	$2\mathrm{PH(ss)c}(lz)$
$6n+4$	$2[c(p_1)c(u_1)+c(p_2)c(u_2)+c(p_3)c(u_3)+c(q_1)c(u_3)$ $+c(q_2)c(u_1)+c(q_3)c(u_2)]$	$2[c(p_1)s(u_1)+c(p_2)s(u_2)+c(p_3)s(u_3)-c(q_1)s(u_3)$ $-c(q_2)s(u_1)-c(q_3)s(u_2)]$
$6n+5$	$-2[s(p_1)s(u_1)+s(p_2)s(u_3)+s(p_3)s(u_2)-s(q_1)s(u_2)$ $-s(q_2)s(u_1)-s(q_3)s(u_3)]$	$2[s(p_1)c(u_1)+s(p_2)c(u_3)+s(p_3)c(u_2)+s(q_1)c(u_2)$ $+s(q_2)c(u_1)+s(q_3)c(u_3)]$

$P6_522$ [No. 179] (enantiomorphous to $P6_122$ [No. 178])

l	A, B
$6n$	as for $P622$ [No. 177]
$6n+1$	as for $l = 6n+5$ in $P6_122$ [No. 178]
$6n+2$	as for $l = 6n+4$ in $P6_122$ [No. 178]
$6n+3$	as for $l = 6n+3$ in $P6_122$ [No. 178]
$6n+4$	as for $l = 6n+2$ in $P6_122$ [No. 178]
$6n+5$	as for $l = 6n+1$ in $P6_122$ [No. 178]

$P6_222$ [No. 180] (enantiomorphous to $P6_422$ [No. 181])

l	A, B
n	as for $P622$ [No. 177]
$3n+1$	as for $l = 6n+2$ in $P6_122$ [No. 178]
$3n+2$	as for $l = 6n+4$ in $P6_122$ [No.178]

$P6_422$ [No. 181] (enantiomorphous to $P6_222$ [No. 180])

l	A, B
$3n$	as for $P622$ [No. 177]
$3n+1$	as for $l = 6n+4$ in $P6_122$ [No. 178]
$3n+2$	as for $l = 6n+2$ in $P6_122$ [No. 178]

$P6_322$ [No. 182]

l	A, B
$2n$	as for $P622$ [No. 177]
$2n+1$	as for $l = 6n+3$ in $P6_122$ [No. 178]

$P6mm$ [No. 183]

hkl	A	B
All	$2\mathrm{PH(cc)c}(lz)$	$2\mathrm{PH(cc)s}(lz)$

$P6cc$ [No. 184]

l	A	B
$2n$	$2\mathrm{PH(cc)c}(lz)$	$2\mathrm{PH(cc)s}(lz)$
$2n+1$	$2\mathrm{MH(cc)c}(lz)$	$2\mathrm{MH(cc)s}(lz)$

Table A1.4.3.6. *Trigonal and hexagonal space groups* (*cont.*)

$P6_3cm$ [No. 185]

l	A	B
$2n$ $2n+1$	2PH(cc)c(lz) −2PH(ss)s(lz)	2PH(cc)s(lz) 2PH(ss)c(lz)

$P6_3mc$ [No. 186]

l	A	B
$2n$ $2n+1$	2PH(cc)c(lz) −2MH(ss)s(lz)	2PH(cc)s(lz) 2MH(ss)c(lz)

$P\bar{6}m2$ [No. 187]

hkl	A	B
All	2PH(cc)c(lz)	2MH(ss)c(lz)

$P\bar{6}c2$ [No. 188]

l	A	B
$2n$ $2n+1$	2PH(cc)c(lz) −2PH(ss)s(lz)	2MH(ss)c(lz) 2MH(cc)s(lz)

$P\bar{6}2m$ [No. 189]

hkl	A	B
All	2PH(cc)c(lz)	2PH(ss)c(lz)

$P\bar{6}2c$ [No. 190]

l	A	B
$2n$ $2n+1$	2PH(cc)c(lz) −2MH(ss)s(lz)	2PH(ss)c(lz) 2MH(cc)s(lz)

$P6/mmm$ [No. 191]

hkl	A	B
All	4PH(cc)c(lz)	0

$P6/mcc$ [No. 192] ($B = 0$ for all h, k, l)

l	A
$2n$ $2n+1$	4PH(cc)c(lz) 4MH(cc)c(lz)

$P6_3/mcm$ [No. 193] ($B = 0$ for all h, k, l)

l	A
$2n$ $2n+1$	4PH(cc)c(lz) −4PH(ss)s(lz)

$P6_3/mmc$ [No. 194] ($B = 0$ for all h, k, l)

l	A
$2n$ $2n+1$	4PH(cc)c(lz) −4MH(ss)s(lz)

Table A1.4.3.7. *Cubic space groups*

The symbols appearing in this table are related to the pqr representation used with the orthorhombic space groups as follows: Each of the symbols defined below is a sum of three pqr terms, where the order of *hkl* is fixed in each of the three terms and that of *xyz* is permuted.

This table and parts of Table A1.4.3.6 (rhombohedral space groups referred to rhombohedral axes) are given in terms of the following two symbols:

$$\mathrm{Epqr} = \mathrm{p}(hx)\mathrm{q}(ky)\mathrm{r}(lz) + \mathrm{p}(hy)\mathrm{q}(kz)\mathrm{r}(lx) + \mathrm{p}(hz)\mathrm{q}(kx)\mathrm{r}(ly) \quad (A1.4.3.7)$$

and

$$\mathrm{Opqr} = \mathrm{p}(hx)\mathrm{q}(kz)\mathrm{r}(ly) + \mathrm{p}(hz)\mathrm{q}(ky)\mathrm{r}(lx) + \mathrm{p}(hy)\mathrm{q}(kx)\mathrm{r}(lz), \quad (A1.4.3.8)$$

where p, q and r can each be a sine or a cosine, and the factor 2π has been absorbed in the abbreviations (see text). As in Tables A1.4.3.1–A1.4.3.6, cosine and sine are abbreviated by c and s, respectively. The permutation of the coordinates is even in Epqr and odd in Opqr.

Conditions for vanishing symbols:

Epqr = Opqr = 0 if at least one of p, q, r is a sine and the index *h*, *k* or *l* in its argument is zero,

$$\mathrm{Eccc} - \mathrm{Occc} = 0 \text{ if } |h| = |k| \text{ (or } |k| = |l| \text{ or } |l| = |h|),$$
$$\mathrm{Esss} - \mathrm{Osss} = 0 \text{ if } |h| = |k| \text{ (or } |k| = |l| \text{ or } |l| = |h|),$$
$$\mathrm{Ecss} - \mathrm{Ocss} = \mathrm{Escc} - \mathrm{Oscc} = 0 \text{ if } |k| = |l|,$$
$$\mathrm{Escs} - \mathrm{Oscs} = \mathrm{Ecsc} - \mathrm{Ocsc} = 0 \text{ if } |l| = |h| \text{ and}$$
$$\mathrm{Essc} - \mathrm{Ossc} = \mathrm{Eccs} - \mathrm{Occs} = 0 \text{ if } |h| = |k|.$$

*P*23 [No. 195]

hkl	*A*	*B*
All	4Eccc	−4Esss

*F*23 [No. 196]

hkl	*A*	*B*
All	16Eccc	−16Esss

*I*23 [No. 197]

hkl	*A*	*B*
All	8Eccc	−8Esss

$P2_13$ [No. 198]

$h+k$	$k+l$	$h+l$	*A*	*B*
$2n$	$2n$	$2n$	4Eccc	−4Esss
$2n$	$2n+1$	$2n+1$	−4Ecss	4Escc
$2n+1$	$2n$	$2n+1$	−4Escs	4Ecsc
$2n+1$	$2n+1$	$2n$	−4Essc	4Eccs

$I2_13$ [No. 199]

$h+k$	$k+l$	$h+l$	*A*	*B*
$2n$	$2n$	$2n$	8Eccc	−8Esss
$2n+1$	$2n$	$2n+1$	−8Escs	8Ecsc
$2n+1$	$2n+1$	$2n$	−8Essc	8Eccs
$2n$	$2n+1$	$2n+1$	−8Ecss	8Escc

$Pm\bar{3}$ [No. 200]

hkl	*A*	*B*
All	8Eccc	0

$Pn\bar{3}$ (Origin 1) [No. 201]

$h+k+l$	*A*	*B*
$2n$	8Eccc	0
$2n+1$	0	−8Esss

Table A1.4.3.7. *Cubic space groups* (*cont.*)

$Pn\overline{3}$ (Origin 2) [No. 201] ($B = 0$ for all h, k, l)

$h + k$	$k + l$	$h + l$	A
$2n$	$2n$	$2n$	8Eccc
$2n$	$2n + 1$	$2n + 1$	−8Essc
$2n + 1$	$2n$	$2n + 1$	−8Ecss
$2n + 1$	$2n + 1$	$2n$	−8Escs

$Fm\overline{3}$ [No. 202]

hkl	A	B
All	32Eccc	0

$Fd\overline{3}$ (Origin 1) [No. 203]

$h + k + l$	A	B
$4n$	32Eccc	0
$4n + 1$	16(Eccc − Esss)	A
$4n + 2$	0	−32Esss
$4n + 3$	16(Eccc + Esss)	$-A$

$Fd\overline{3}$ (Origin 2) [No. 203] ($B = 0$ for all h, k, l)

$h + k$	$k + l$	$h + l$	A
$4n$	$4n$	$4n$	32Eccc
$4n$	$4n + 2$	$4n + 2$	−32Essc
$4n + 2$	$4n$	$4n + 2$	−32Ecss
$4n + 2$	$4n + 2$	$4n$	−32Escs
$4n + 2$	$4n + 2$	$4n + 2$	−16(Eccc + Ecss + Escs + Essc)
$4n + 2$	$4n$	$4n$	16(Eccc − Ecss − Escs + Essc)
$4n$	$4n + 2$	$4n$	16(Eccc + Ecss − Escs − Essc)
$4n$	$4n$	$4n + 2$	16(Eccc − Ecss + Escs −Essc)

$Im\overline{3}$ [No. 204]

hkl	A	B
All	16Eccc	0

$Pa\overline{3}$ [No. 205] ($B = 0$ for all h, k, l)

$h + k$	$k + l$	$h + l$	A
$2n$	$2n$	$2n$	8Eccc
$2n$	$2n + 1$	$2n + 1$	−8Ecss
$2n + 1$	$2n$	$2n + 1$	−8Escs
$2n + 1$	$2n + 1$	$2n$	−8Essc

$Ia\overline{3}$ [No. 206] ($B = 0$ for all h, k, l)

$h + k$	$k + l$	$h + l$	A
$2n$	$2n$	$2n$	16Eccc
$2n$	$2n + 1$	$2n + 1$	−16Ecss
$2n + 1$	$2n$	$2n + 1$	−16Escs
$2n + 1$	$2n + 1$	$2n$	−16Essc

$P432$ [No. 207]

hkl	A	B
All	4(Eccc + Occc)	−4(Esss − Osss)

Table A1.4.3.7. *Cubic space groups* (*cont.*)

$P4_232$ [No. 208]

$h+k+l$	A	B
$2n$	4(Eccc + Occc)	−4(Esss − Osss)
$2n+1$	4(Eccc − Occc)	−4(Esss + Osss)

$F432$ [No. 209]

hkl	A	B
All	16(Eccc + Occc)	−16(Esss − Osss)

$F4_132$ [No. 210]

$h+k+l$	A	B
$4n$	16(Eccc + Occc)	−16(Esss − Osss)
$4n+1$	16(Eccc − Osss)	−16(Esss − Occc)
$4n+2$	16(Eccc − Occc)	−16(Esss + Osss)
$4n+3$	16(Eccc + Osss)	−16(Esss + Occc)

$I432$ [No. 211]

hkl	A	B
All	8(Eccc + Occc)	−8(Esss − Osss)

$P4_332$ [No. 212] (enantiomorphous to $P4_132$ [No. 213])

$h+k$	$k+l$	$h+l$	$h+k+l$	A	B
$2n$	$2n$	$2n$	$4n$	4(Eccc + Occc)	−4(Esss − Osss)
$2n$	$2n+1$	$2n+1$	$4n$	−4(Ecss + Oscs)	4(Escc − Ocsc)
$2n+1$	$2n$	$2n+1$	$4n$	−4(Escs + Ossc)	4(Ecsc − Occs)
$2n+1$	$2n+1$	$2n$	$4n$	−4(Essc + Ocss)	4(Eccs − Oscc)
$2n$	$2n$	$2n$	$4n+1$	4(Eccc − Osss)	−4(Esss − Occc)
$2n$	$2n+1$	$2n+1$	$4n+1$	−4(Ecss − Ocsc)	4(Escc − Oscs)
$2n+1$	$2n$	$2n+1$	$4n+1$	−4(Escs − Occs)	4(Ecsc − Ossc)
$2n+1$	$2n+1$	$2n$	$4n+1$	−4(Essc − Oscc)	4(Eccs − Ocss)
$2n$	$2n$	$2n$	$4n+2$	4(Eccc − Occc)	−4(Esss + Osss)
$2n$	$2n+1$	$2n+1$	$4n+2$	−4(Ecss − Oscs)	4(Escc + Ocsc)
$2n+1$	$2n$	$2n+1$	$4n+2$	−4(Escs − Ossc)	4(Ecsc + Occs)
$2n+1$	$2n+1$	$2n$	$4n+2$	−4(Essc − Ocss)	4(Eccs + Oscc)
$2n$	$2n$	$2n$	$4n+3$	4(Eccc + Osss)	−4(Esss + Occc)
$2n$	$2n+1$	$2n+1$	$4n+3$	−4(Ecss + Ocsc)	4(Escc + Oscs)
$2n+1$	$2n$	$2n+1$	$4n+3$	−4(Escs + Occs)	4(Ecsc + Ossc)
$2n+1$	$2n+1$	$2n$	$4n+3$	−4(Essc + Oscc)	4(Eccs + Ocss)

$P4_132$ [No. 213] (enantiomorphous to $P4_332$ [No. 212])

h	k	l	$h+k+l$	A	B
$2n$	$2n$	$2n$	$4n$	4(Eccc + Occc)	−4(Esss − Osss)
$2n$	$2n+1$	$2n+1$	$4n$	−4(Escs + Ossc)	4(Ecsc − Occs)
$2n+1$	$2n$	$2n+1$	$4n$	−4(Essc + Ocss)	4(Eccs − Oscc)
$2n+1$	$2n+1$	$2n$	$4n$	−4(Ecss + Oscs)	4(Escc − Ocsc)
$2n+1$	$2n+1$	$2n+1$	$4n+1$	4(Eccc + Osss)	−4(Esss + Occc)
$2n$	$2n$	$2n+1$	$4n+1$	−4(Ecss + Ocsc)	4(Escc + Oscs)
$2n+1$	$2n$	$2n$	$4n+1$	−4(Escs + Occs)	4(Ecsc + Ossc)
$2n$	$2n+1$	$2n$	$4n+1$	−4(Essc + Oscc)	4(Eccs + Ocss)
$2n$	$2n$	$2n$	$4n+2$	4(Eccc − Occc)	−4(Esss + Osss)
$2n$	$2n+1$	$2n+1$	$4n+2$	−4(Escs − Ossc)	4(Ecsc + Occs)
$2n+1$	$2n$	$2n+1$	$4n+2$	−4(Essc − Ocss)	4(Eccs + Oscc)

Table A1.4.3.7. *Cubic space groups* (*cont.*)

h	k	l	$h+k+l$	A	B
$2n+1$	$2n+1$	$2n$	$4n+2$	−4(Ecss − Oscs)	4(Escc + Ocsc)
$2n+1$	$2n+1$	$2n+1$	$4n+3$	4(Eccc − Osss)	−4(Esss − Occc)
$2n$	$2n$	$2n+1$	$4n+3$	−4(Ecss − Ocsc)	4(Escc − Oscs)
$2n+1$	$2n$	$2n$	$4n+3$	−4(Escs − Occs)	4(Ecsc − Ossc)
$2n$	$2n+1$	$2n$	$4n+3$	−4(Essc − Oscc)	4(Eccs − Ocss)

$I4_132$ [No. 214]

h	k	l	$h+k+l$	A	B
$2n$	$2n$	$2n$	$4n$	8(Eccc + Occc)	−8(Esss − Osss)
$2n$	$2n+1$	$2n+1$	$4n$	−8(Escs + Ossc)	8(Ecsc − Occs)
$2n+1$	$2n$	$2n+1$	$4n$	−8(Essc + Ocss)	8(Eccs − Oscc)
$2n+1$	$2n+1$	$2n$	$4n$	−8(Ecss + Oscs)	8(Escc − Ocsc)
$2n$	$2n$	$2n$	$4n+2$	8(Eccc − Occc)	−8(Esss + Osss)
$2n$	$2n+1$	$2n+1$	$4n+2$	−8(Escs − Ossc)	8(Ecsc + Occs)
$2n+1$	$2n$	$2n+1$	$4n+2$	−8(Essc − Ocss)	8(Eccs + Oscc)
$2n+1$	$2n+1$	$2n$	$4n+2$	−8(Ecss − Oscs)	8(Escc + Ocsc)

$P\bar{4}3m$ [No. 215]

hkl	A	B
All	4(Eccc + Occc)	−4(Esss + Osss)

$F\bar{4}3m$ [No. 216]

hkl	A	B
All	16(Eccc + Occc)	−16(Esss + Osss)

$I\bar{4}3m$ [No. 217]

hkl	A	B
All	8(Eccc + Occc)	−8(Esss +Osss)

$P\bar{4}3n$ [No. 218]

$h+k+l$	A	B
$2n$	4(Eccc + Occc)	−4(Esss + Osss)
$2n+1$	4(Eccc − Occc)	−4(Esss − Osss)

$F\bar{4}3c$ [No. 219]

$h+k+l$	A	B
$2n$	16(Eccc + Occc)	−16(Esss + Osss)
$2n+1$	16(Eccc − Occc)	−16(Esss − Osss)

$I\bar{4}3d$ [No. 220]

h	k	l	$h+k+l$	A	B
$2n$	$2n$	$2n$	$4n$	8(Eccc + Occc)	−8(Esss + Osss)
$2n$	$2n+1$	$2n+1$	$4n$	−8(Escs + Ossc)	8(Ecsc + Occs)
$2n+1$	$2n$	$2n+1$	$4n$	−8(Essc + Ocss)	8(Eccs + Oscc)
$2n+1$	$2n+1$	$2n$	$4n$	−8(Ecss + Oscs)	8(Escc + Ocsc)
$2n$	$2n$	$2n$	$4n+2$	8(Eccc − Occc)	−8(Esss − Osss)
$2n$	$2n+1$	$2n+1$	$4n+2$	−8(Escs − Ossc)	8(Ecsc − Occs)
$2n+1$	$2n$	$2n+1$	$4n+2$	−8(Essc − Ocss)	8(Eccs − Oscc)
$2n+1$	$2n+1$	$2n$	$4n+2$	−8(Ecss − Oscs)	8(Escc −Ocsc)

Table A1.4.3.7. *Cubic space groups* (*cont.*)

$Pm\bar{3}m$ [No. 221]

hkl	*A*	*B*
All	8(Eccc + Occc)	0

$Pn\bar{3}n$ (Origin 1) [No. 222]

$h+k+l$	*A*	*B*
$2n$	8(Eccc + Occc)	0
$2n+1$	0	−8(Esss − Osss)

$Pn\bar{3}n$ (Origin 2) [No. 222] ($B = 0$ for all h, k, l)

h	*k*	*l*	*A*
$2n$	$2n$	$2n$	8(Eccc + Occc)
$2n$	$2n+1$	$2n+1$	−8(Ecss + Ocss)
$2n+1$	$2n$	$2n+1$	−8(Escs + Oscs)
$2n+1$	$2n+1$	$2n$	−8(Essc + Ossc)
$2n+1$	$2n+1$	$2n+1$	8(Eccc − Occc)
$2n+1$	$2n$	$2n$	−8(Ecss − Ocss)
$2n$	$2n+1$	$2n$	−8(Escs − Oscs)
$2n$	$2n$	$2n+1$	−8(Essc − Ossc)

$Pm\bar{3}n$ [No. 223] ($B = 0$ for all h, k, l)

$h+k+l$	*A*
$2n$	8(Eccc + Occc)
$2n+1$	8(Eccc − Occc)

$Pn\bar{3}m$ (Origin 1) [No. 224]

$h+k+l$	*A*	*B*
$2n$	8(Eccc + Occc)	0
$2n+1$	0	−8(Esss + Osss)

$Pn\bar{3}m$ (Origin 2) [No. 224] ($B = 0$ for all h, k, l)

$h+k$	$k+l$	$h+l$	*A*
$2n$	$2n$	$2n$	8(Eccc + Occc)
$2n$	$2n+1$	$2n+1$	−8(Essc + Ossc)
$2n+1$	$2n$	$2n+1$	−8(Ecss + Ocss)
$2n+1$	$2n+1$	$2n$	−8(Escs + Oscs)

$Fm\bar{3}m$ [No. 225]

hkl	*A*	*B*
All	32(Eccc + Occc)	0

$Fm\bar{3}c$ [No. 226] ($B = 0$ for all h, k, l)

$h+k+l$	*A*
$2n$	32(Eccc + Occc)
$2n+1$	32(Eccc − Occc)

Table A1.4.3.7. *Cubic space groups* (*cont.*)

$Fd\overline{3}m$ (Origin 1) [No. 227]

$h+k+l$	A	B
$4n$	32(Eccc + Occc)	0
$4n+1$	16(Eccc − Esss + Occc − Osss)	A
$4n+2$	0	−32(Esss + Osss)
$4n+3$	16(Eccc + Esss + Occc + Osss)	$-A$

$Fd\overline{3}m$ (Origin 2) [No. 227] ($B = 0$ for all h, k, l)

$h+k$	$k+l$	$h+l$	A
$4n$	$4n$	$4n$	32(Eccc + Occc)
$4n$	$4n+2$	$4n+2$	−32(Essc + Ossc)
$4n+2$	$4n$	$4n+2$	−32(Ecss + Ocss)
$4n+2$	$4n+2$	$4n$	−32(Escs + Oscs)
$4n+2$	$4n+2$	$4n+2$	−16(Eccc + Ecss + Escs + Essc + Occc + Ocss + Oscs + Ossc)
$4n+2$	$4n$	$4n$	16(Eccc − Ecss − Escs + Essc + Occc − Ocss − Oscs + Ossc)
$4n$	$4n+2$	$4n$	16(Eccc + Ecss − Escs − Essc + Occc + Ocss − Oscs − Ossc)
$4n$	$4n$	$4n+2$	16(Eccc − Ecss + Escs − Essc + Occc − Ocss + Oscs − Ossc)

$Fd\overline{3}c$ (Origin 1) [No. 228]

$h+k+l$	A	B
$4n$	32(Eccc + Occc)	0
$4n+1$	16(Eccc + Esss − Occc − Osss)	$-A$
$4n+2$	0	−32(Esss + Osss)
$4n+3$	16(Eccc − Esss − Occc + Osss)	A

$Fd\overline{3}c$ (Origin 2) [No. 228] ($B = 0$ for all h, k, l)

$h+k$	$k+l$	$h+l$	A
$4n$	$4n$	$4n$	32(Eccc + Occc)
$4n$	$4n+2$	$4n+2$	−32(Essc + Ossc)
$4n+2$	$4n$	$4n+2$	−32(Ecss + Ocss)
$4n+2$	$4n+2$	$4n$	−32(Escs + Oscs)
$4n+2$	$4n+2$	$4n+2$	−16(Eccc + Ecss + Escs + Essc − Occc − Ocss − Oscs −Ossc)
$4n+2$	$4n$	$4n$	16(Eccc − Ecss − Escs + Essc − Occc + Ocss + Oscs − Ossc)
$4n$	$4n+2$	$4n$	16(Eccc + Ecss − Escs − Essc − Occc − Ocss + Oscs + Ossc)
$4n$	$4n$	$4n+2$	16(Eccc − Ecss + Escs − Essc −Occc + Ocss − Oscs + Ossc)

$Im\overline{3}m$ [No. 229]

hkl	A	B
All	16(Eccc + Occc)	0

$Ia\overline{3}d$ [No. 230] ($B = 0$ for all h, k, l)

h	k	l	$h+k+l$	A
$2n$	$2n$	$2n$	$4n$	16(Eccc + Occc)
$2n$	$2n+1$	$2n+1$	$4n$	−16(Escs + Ossc)
$2n+1$	$2n$	$2n+1$	$4n$	−16(Essc + Ocss)
$2n+1$	$2n+1$	$2n$	$4n$	−16(Ecss + Oscs)
$2n$	$2n$	$2n$	$4n+2$	16(Eccc − Occc)
$2n$	$2n+1$	$2n+1$	$4n+2$	−16(Escs − Ossc)
$2n+1$	$2n$	$2n+1$	$4n+2$	−16(Essc − Ocss)
$2n+1$	$2n+1$	$2n$	$4n+2$	−16(Ecss − Oscs)

Appendix 1.4.4.

Crystallographic space groups in reciprocal space

Table A1.4.4.1. *Crystallographic space groups in reciprocal space*

The table entries are described in detail in Section 1.4.4.1. The general format of an entry is

$$(n)\ \mathbf{h}^T\boldsymbol{P}_n : -\mathbf{h}^T\mathbf{t}_n$$

or

$$(n)\ \mathbf{h}^T\boldsymbol{P}_n : ,$$

according as the phase-shift part of the entry is nonzero or zero modolo 2π, respectively.

Notes:

(1) For centrosymmetric space groups with the centre located at the unit-cell origin only those entries are given which correspond to symmetry operations not related by inversion. If the origin in such space groups is chosen elsewhere, all the entries corresponding to the operations of the point group are presented.

(2) For trigonal and hexagonal space groups referred to hexagonal axes the Miller–Bravais indices *hkil* are employed, and for the rhombohedral space groups referred to rhombohedral axes the indices are denoted by *hkl* (*cf. IT* I, 1952).

Point group: 1 Triclinic Laue group: $\bar{1}$

$P1$ No. 1 (1)
(1) hkl:

Point group: $\bar{1}$ Triclinic Laue group: $\bar{1}$

$P\bar{1}$ No. 2 (2)
(1) hkl:

Point group: 2 Monoclinic Laue group: 2/*m*

$P2$ $P121$ Unique axis *b* No. 3 (3)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$P2$ $P112$ Unique axis *c* No. 3 (4)
(1) hkl: (2) $\bar{h}\bar{k}l$:

$P2_1$ $P12_11$ Unique axis *b* No. 4 (5)
(1) hkl: (2) $\bar{h}k\bar{l}$: $-010/2$

$P2_1$ $P112_1$ Unique axis *c* No. 4 (6)
(1) hkl: (2) $\bar{h}\bar{k}l$: $-001/2$

$C2$ $C121$ Unique axis *b* No. 5 (7)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2$ $A121$ Unique axis *b* No. 5 (8)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2$ $I121$ Unique axis *b* No. 5 (9)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2$ $A112$ Unique axis *c* No. 5 (10)
(1) hkl: (2) $\bar{h}\bar{k}l$:

$C2$ $B112$ Unique axis *c* No. 5 (11)
(1) hkl: (2) $\bar{h}\bar{k}l$:

$C2$ $I112$ Unique axis *c* No. 5 (12)
(1) hkl: (2) $\bar{h}\bar{k}l$:

Point group: *m* Monoclinic Laue group: 2/*m*

Pm $P1m1$ Unique axis *b* No. 6 (13)
(1) hkl: (2) $h\bar{k}l$:

Pm $P11m$ Unique axis *c* No. 6 (14)
(1) hkl: (2) $hk\bar{l}$:

Pc $P1c1$ Unique axis *b* No. 7 (15)
(1) hkl: (2) $h\bar{k}l$: $-001/2$

Pc $P1n1$ Unique axis *b* No. 7 (16)
(1) hkl: (2) $h\bar{k}l$: $-101/2$

Pc $P1a1$ Unique axis *b* No. 7 (17)
(1) hkl: (2) $h\bar{k}l$: $-100/2$

Pc $P11a$ Unique axis *c* No. 7 (18)
(1) hkl: (2) $hk\bar{l}$: $-100/2$

Pc $P11n$ Unique axis *c* No. 7 (19)
(1) hkl: (2) $hk\bar{l}$: $-110/2$

Pc $P11b$ Unique axis *c* No. 7 (20)
(1) hkl: (2) $hk\bar{l}$: $-010/2$

Cm $C1m1$ Unique axis *b* No. 8 (21)
(1) hkl: (2) $h\bar{k}l$:

Cm $A1m1$ Unique axis *b* No. 8 (22)
(1) hkl: (2) $h\bar{k}l$:

Cm $I1m1$ Unique axis *b* No. 8 (23)
(1) hkl: (2) $h\bar{k}l$:

Cm $A11m$ Unique axis *c* No. 8 (24)
(1) hkl: (2) $hk\bar{l}$:

Cm $B11m$ Unique axis *c* No. 8 (25)
(1) hkl: (2) $hk\bar{l}$:

Cm $I11m$ Unique axis *c* No. 8 (26)
(1) hkl: (2) $hk\bar{l}$:

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

Cc $C1c1$ Unique axis *b* No. 9 (27)
(1) hkl: (2) $h\bar{k}l$: −001/2

Cc $A1n1$ Unique axis *b* No. 9 (28)
(1) hkl: (2) $h\bar{k}l$: −101/2

Cc $I1a1$ Unique axis *b* No. 9 (29)
(1) hkl: (2) $h\bar{k}l$: −100/2

Cc $A11a$ Unique axis *c* No. 9 (30)
(1) hkl: (2) $hk\bar{l}$: −100/2

Cc $B11n$ Unique axis *c* No. 9 (31)
(1) hkl: (2) $hk\bar{l}$: −110/2

Cc $I11b$ Unique axis *c* No. 9 (32)
(1) hkl: (2) $hk\bar{l}$: −010/2

Point group: 2/*m* **Monoclinic** **Laue group: 2/*m***

$P2/m$ $P12/m1$ Unique axis *b* No. 10 (33)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$P2/m$ $P112/m$ Unique axis *c* No. 10 (34)
(1) hkl: (2) $\overline{hk}l$:

$P2_1/m$ $P12_1/m1$ Unique axis *b* No. 11 (35)
(1) hkl: (2) $\bar{h}k\bar{l}$: −010/2

$P2_1/m$ $P112_1/m$ Unique axis *c* No. 11 (36)
(1) hkl: (2) $\overline{hk}l$: −001/2

$C2/m$ $C12/m1$ Unique axis *b* No. 12 (37)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2/m$ $A12/m1$ Unique axis *b* No. 12 (38)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2/m$ $I12/m1$ Unique axis *b* No. 12 (39)
(1) hkl: (2) $\bar{h}k\bar{l}$:

$C2/m$ $A112/m$ Unique axis *c* No. 12 (40)
(1) hkl: (2) $\overline{hk}l$:

$C2/m$ $B112/m$ Unique axis *c* No. 12 (41)
(1) hkl: (2) $\overline{hk}l$:

$C2/m$ $I112/m$ Unique axis *c* No. 12 (42)
(1) hkl: (2) $\overline{hk}l$:

$P2/c$ $P12/c1$ Unique axis *b* No. 13 (43)
(1) hkl: (2) $\bar{h}k\bar{l}$: −001/2

$P2/c$ $P12/n1$ Unique axis *b* No. 13 (44)
(1) hkl: (2) $\bar{h}k\bar{l}$: −101/2

$P2/c$ $P12/a1$ Unique axis *b* No. 13 (45)
(1) hkl: (2) $\bar{h}k\bar{l}$: −100/2

$P2/c$ $P112/a$ Unique axis *c* No. 13 (46)
(1) hkl: (2) $\overline{hk}l$: −100/2

$P2/c$ $P112/n$ Unique axis *c* No. 13 (47)
(1) hkl: (2) $\overline{hk}l$: −110/2

$P2/c$ $P112/b$ Unique axis *c* No. 13 (48)
(1) hkl: (2) $\overline{hk}l$: −010/2

$P2_1/c$ $P12_1/c1$ Unique axis *b* No. 14 (49)
(1) hkl: (2) $\bar{h}k\bar{l}$: −011/2

$P2_1/c$ $P12_1/n1$ Unique axis *b* No. 14 (50)
(1) hkl: (2) $\bar{h}k\bar{l}$: −111/2

$P2_1/c$ $P12_1/a1$ Unique axis *b* No. 14 (51)
(1) hkl: (2) $\bar{h}k\bar{l}$: −110/2

$P2_1/c$ $P112_1/a$ Unique axis *c* No. 14 (52)
(1) hkl: (2) $\overline{hk}l$: −101/2

$P2_1/c$ $P112_1/n$ Unique axis *c* No. 14 (53)
(1) hkl: (2) $\overline{hk}l$: −111/2

$P2_1/c$ $P112_1/b$ Unique axis *c* No. 14 (54)
(1) hkl: (2) $\overline{hk}l$: −011/2

$C2/c$ $C12/c1$ Unique axis *b* No. 15 (55)
(1) hkl: (2) $\bar{h}k\bar{l}$: −001/2

$C2/c$ $A12/n1$ Unique axis *b* No. 15 (56)
(1) hkl: (2) $\bar{h}k\bar{l}$: −101/2

$C2/c$ $I12/a1$ Unique axis *b* No. 15 (57)
(1) hkl: (2) $\bar{h}k\bar{l}$: −100/2

$C2/c$ $A112/a$ Unique axis *c* No. 15 (58)
(1) hkl: (2) $\overline{hk}l$: −100/2

$C2/c$ $B112/n$ Unique axis *c* No. 15 (59)
(1) hkl: (2) $\overline{hk}l$: −110/2

$C2/c$ $I112/b$ Unique axis *c* No. 15 (60)
(1) hkl: (2) $\overline{hk}l$: −010/2

Point group: 222 **Orthorhombic** **Laue group: *mmm***

$P222$ No. 16 (61)
(1) hkl: (2) $\overline{hk}l$: (3) $\bar{h}k\bar{l}$: (4) $h\overline{kl}$:

$P222_1$ No. 17 (62)
(1) hkl: (2) $\overline{hk}l$: −001/2 (3) $\bar{h}k\bar{l}$: −001/2 (4) $h\overline{kl}$:

$P2_12_12$ No. 18 (63)
(1) hkl: (2) $\overline{hk}l$: (3) $\bar{h}k\bar{l}$: −110/2 (4) $h\overline{kl}$: −110/2

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P2_12_12_1$ No. 19 (64)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
$C222_1$ No. 20 (65)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$:
$C222$ No. 21 (66)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
$F222$ No. 22 (67)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
$I222$ No. 23 (68)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
$I2_12_12_1$ No. 24 (69)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2

Point group: *mm*2 Orthorhombic Laue group: *mmm*

$Pmm2$ No. 25 (70)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$:	(4) $\bar{h}kl$:
$Pmc2_1$ No. 26 (71)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $h\bar{k}l$: −001/2	(4) $\bar{h}kl$:
$Pcc2$ No. 27 (72)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −001/2	(4) $\bar{h}kl$: −001/2
$Pma2$ No. 28 (73)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −100/2	(4) $\bar{h}kl$: −100/2
$Pca2_1$ No. 29 (74)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $h\bar{k}l$: −100/2	(4) $\bar{h}kl$: −101/2
$Pnc2$ No. 30 (75)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −011/2	(4) $\bar{h}kl$: −011/2
$Pmn2_1$ No. 31 (76)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $h\bar{k}l$: −101/2	(4) $\bar{h}kl$:
$Pba2$ No. 32 (77)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −110/2	(4) $\bar{h}kl$: −110/2
$Pna2_1$ No. 33 (78)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $h\bar{k}l$: −110/2	(4) $\bar{h}kl$: −111/2
$Pnn2$ No. 34 (79)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −111/2	(4) $\bar{h}kl$: −111/2
$Cmm2$ No. 35 (80)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$:	(4) $\bar{h}kl$:
$Cmc2_1$ No. 36 (81)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $h\bar{k}l$: −001/2	(4) $\bar{h}kl$:
$Ccc2$ No. 37 (82)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −001/2	(4) $\bar{h}kl$: −001/2
$Amm2$ No. 38 (83)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$:	(4) $\bar{h}kl$:
$Abm2$ No. 39 (84)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −010/2	(4) $\bar{h}kl$: −010/2
$Ama2$ No. 40 (85)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −100/2	(4) $\bar{h}kl$: −100/2
$Aba2$ No. 41 (86)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −110/2	(4) $\bar{h}kl$: −110/2
$Fmm2$ No. 42 (87)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$:	(4) $\bar{h}kl$:
$Fdd2$ No. 43 (88)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −313/4	(4) $\bar{h}kl$: −133/4
$Imm2$ No. 44 (89)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$:	(4) $\bar{h}kl$:
$Iba2$ No. 45 (90)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −110/2	(4) $\bar{h}kl$: −110/2
$Ima2$ No. 46 (91)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $h\bar{k}l$: −100/2	(4) $\bar{h}kl$: −100/2

Point group: *mmm* Orthorhombic Laue group: *mmm*

$Pmmm$ No. 47 (92)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
$Pnnn$ Origin 1 No. 48 (93)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) $\bar{h}\bar{k}\bar{l}$: −111/2	(6) $hk\bar{l}$: −111/2	(7) $h\bar{k}l$: −111/2	(8) $\bar{h}kl$: −111/2
$Pnnn$ Origin 2 No. 48 (94)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −101/2	(4) $h\bar{k}\bar{l}$: −011/2
$Pccm$ No. 49 (95)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$: −001/2
$Pban$ Origin 1 No. 50 (96)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) $\bar{h}\bar{k}\bar{l}$: −110/2	(6) $hk\bar{l}$: −110/2	(7) $h\bar{k}l$: −110/2	(8) $\bar{h}kl$: −110/2
$Pban$ Origin 2 No. 50 (97)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −100/2	(4) $h\bar{k}\bar{l}$: −010/2
$Pmma$ No. 51 (98)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −100/2	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$: −100/2
$Pnna$ No. 52 (99)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −100/2	(3) $\bar{h}k\bar{l}$: −111/2	(4) $h\bar{k}\bar{l}$: −011/2

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

Pmna No. 53 (100)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −101/2	(4) $h\bar{k}\bar{l}$:
Pcca No. 54 (101)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −100/2	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$: −101/2
Pbam No. 55 (102)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −110/2
Pccn No. 56 (103)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −101/2
Pbcm No. 57 (104)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −010/2
Pnnm No. 58 (105)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −111/2	(4) $h\bar{k}\bar{l}$: −111/2
Pmmn Origin 1 No. 59 (106)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −110/2
(5) $\bar{h}\bar{k}\bar{l}$: −110/2	(6) $hk\bar{l}$: −110/2	(7) $h\bar{k}l$:	(8) $\bar{h}kl$:
Pmmn Origin 2 No. 59 (107)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −010/2	(4) $h\bar{k}\bar{l}$: −100/2
Pbcn No. 60 (108)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$: −110/2
Pbca No. 61 (109)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
Pnma No. 62 (110)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −010/2	(4) $h\bar{k}\bar{l}$: −111/2
Cmcm No. 63 (111)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$:
Cmca No. 64 (112)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −011/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$:
Cmmm No. 65 (113)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
Cccm No. 66 (114)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$: −001/2
Cmma No. 67 (115)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −010/2	(3) $\bar{h}k\bar{l}$: −010/2	(4) $h\bar{k}\bar{l}$:
Ccca Origin 1 No. 68 (116)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$: −110/2
(5) $\bar{h}\bar{k}\bar{l}$: −011/2	(6) $hk\bar{l}$: −101/2	(7) $h\bar{k}l$: −011/2	(8) $\bar{h}kl$: −101/2
Ccca Origin 2 No. 68 (117)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −100/2	(3) $\bar{h}k\bar{l}$: −001/2	(4) $h\bar{k}\bar{l}$: −101/2

Fmmm No. 69 (118)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
Fddd Origin 1 No. 70 (119)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) $\bar{h}\bar{k}\bar{l}$: −111/4	(6) $hk\bar{l}$: −111/4	(7) $h\bar{k}l$: −111/4	(8) $\bar{h}kl$: −111/4
Fddd Origin 2 No. 70 (120)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −330/4	(3) $\bar{h}k\bar{l}$: −303/4	(4) $h\bar{k}\bar{l}$: −033/4
Immm No. 71 (121)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
Ibam No. 72 (122)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −110/2
Ibca No. 73 (123)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
Imma No. 74 (124)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −010/2	(3) $\bar{h}k\bar{l}$: −010/2	(4) $h\bar{k}\bar{l}$:

Point group: 4 Tetragonal Laue group: 4/*m*			
*P*4 No. 75 (125)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
$P4_1$ No. 76 (126)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −001/4	(4) $\bar{k}hl$: −003/4
$P4_2$ No. 77 (127)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
$P4_3$ No. 78 (128)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −003/4	(4) $\bar{k}hl$: −001/4
*I*4 No. 79 (129)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
$I4_1$ No. 80 (130)			
(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4

Point group: $\bar{4}$ Tetragonal Laue group: 4/*m*			
$P\bar{4}$ No. 81 (131)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
$I\bar{4}$ No. 82 (132)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:

Point group: 4/*m* Tetragonal Laue group: 4/*m*			
$P4/m$ No. 83 (133)			
(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P4_2/m$ No. 84 (134)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2

$P4/n$ Origin 1 No. 85 (135)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −110/2	(4) $\bar{k}hl$: −110/2
(5) $\bar{h}\bar{k}\bar{l}$: −110/2	(6) $hk\bar{l}$: −110/2	(7) $\bar{k}h\bar{l}$:	(8) $k\bar{h}\bar{l}$:

$P4/n$ Origin 2 No. 85 (136)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −100/2	(4) $\bar{k}hl$: −010/2

$P4_2/n$ Origin 1 No. 86 (137)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}\bar{k}\bar{l}$: −111/2	(6) $hk\bar{l}$: −111/2	(7) $\bar{k}h\bar{l}$:	(8) $k\bar{h}\bar{l}$:

$P4_2/n$ Origin 2 No. 86 (138)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −011/2	(4) $\bar{k}hl$: −101/2

$I4/m$ No. 87 (139)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:

$I4_1/a$ Origin 1 No. 88 (140)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $\bar{h}\bar{k}\bar{l}$: −021/4	(6) $hk\bar{l}$: −203/4	(7) $\bar{k}h\bar{l}$:	(8) $k\bar{h}\bar{l}$: −111/2

$I4_1/a$ Origin 2 No. 88 (141)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $k\bar{h}l$: −311/4	(4) $\bar{k}hl$: −333/4

Point group: 422 Tetragonal Laue group: 4/*mmm*

$P422$ No. 89 (142)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$P42_12$ No. 90 (143)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −110/2	(4) $\bar{k}hl$: −110/2
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\bar{k}\bar{l}$: −110/2	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$P4_122$ No. 91 (144)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −001/4	(4) $\bar{k}hl$: −003/4
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$: −001/2	(7) $kh\bar{l}$: −003/4	(8) $\bar{k}\bar{h}\bar{l}$: −001/4

$P4_12_12$ No. 92 (145)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −221/4	(4) $\bar{k}hl$: −223/4
(5) $\bar{h}k\bar{l}$: −221/4	(6) $h\bar{k}\bar{l}$: −223/4	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$P4_222$ No. 93 (146)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$P4_22_12$ No. 94 (147)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\bar{k}\bar{l}$: −111/2	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$P4_322$ No. 95 (148)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −003/4	(4) $\bar{k}hl$: −001/4
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$: −001/2	(7) $kh\bar{l}$: −001/4	(8) $\bar{k}\bar{h}\bar{l}$: −003/4

$P4_32_12$ No. 96 (149)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −001/2	(3) $k\bar{h}l$: −223/4	(4) $\bar{k}hl$: −221/4
(5) $\bar{h}k\bar{l}$: −223/4	(6) $h\bar{k}\bar{l}$: −221/4	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$I422$ No. 97 (150)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$I4_122$ No. 98 (151)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $\bar{h}k\bar{l}$: −203/4	(6) $h\bar{k}\bar{l}$: −021/4	(7) $kh\bar{l}$: −111/2	(8) $\bar{k}\bar{h}\bar{l}$:

Point group: 4*mm* Tetragonal Laue group: 4/*mmm*

$P4mm$ No. 99 (152)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$:	(6) $\bar{h}kl$:	(7) $\bar{k}\bar{h}l$:	(8) khl:

$P4bm$ No. 100 (153)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$: −110/2	(6) $\bar{h}kl$: −110/2	(7) $\bar{k}\bar{h}l$: −110/2	(8) khl: −110/2

$P4_2cm$ No. 101 (154)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −001/2	(7) $\bar{k}\bar{h}l$:	(8) khl:

$P4_2nm$ No. 102 (155)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $h\bar{k}l$: −111/2	(6) $\bar{h}kl$: −111/2	(7) $\bar{k}\bar{h}l$:	(8) khl:

$P4cc$ No. 103 (156)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −001/2	(7) $\bar{k}\bar{h}l$: −001/2	(8) khl: −001/2

$P4nc$ No. 104 (157)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$: −111/2	(6) $\bar{h}kl$: −111/2	(7) $\bar{k}\bar{h}l$: −111/2	(8) khl: −111/2

$P4_2mc$ No. 105 (158)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $h\bar{k}l$:	(6) $\bar{h}kl$:	(7) $\bar{k}\bar{h}l$: −001/2	(8) khl: −001/2

$P4_2bc$ No. 106 (159)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $h\bar{k}l$: −110/2	(6) $\bar{h}kl$: −110/2	(7) $\bar{k}\bar{h}l$: −111/2	(8) khl: −111/2

$I4mm$ No. 107 (160)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$:	(6) $\bar{h}kl$:	(7) $\bar{k}\bar{h}l$:	(8) khl:

$I4cm$ No. 108 (161)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −001/2	(7) $\bar{k}\bar{h}l$: −001/2	(8) khl: −001/2

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$I4_1md$ No. 109 (162)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $h\bar{k}l$:	(6) $\bar{h}kl$: −111/2	(7) $\bar{k}\bar{h}l$: −203/4	(8) khl: −021/4

$I4_1cd$ No. 110 (163)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −110/2	(7) $\bar{k}\bar{h}l$: −201/4	(8) khl: −023/4

Point group: $\bar{4}2m$ Tetragonal Laue group: 4/*mmm*

$P\bar{4}2m$ No. 111 (164)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $\bar{k}\bar{h}l$:	(8) khl:

$P\bar{4}2c$ No. 112 (165)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$: −001/2	(6) $h\bar{k}\bar{l}$: −001/2	(7) $\bar{k}\bar{h}l$: −001/2	(8) khl: −001/2

$P\bar{4}2_1m$ No. 113 (166)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\bar{k}\bar{l}$: −110/2	(7) $\bar{k}\bar{h}l$: −110/2	(8) khl: −110/2

$P\bar{4}2_1c$ No. 114 (167)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\bar{k}\bar{l}$: −111/2	(7) $\bar{k}\bar{h}l$: −111/2	(8) khl: −111/2

$P\bar{4}m2$ No. 115 (168)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$:	(6) $\bar{h}kl$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$P\bar{4}c2$ No. 116 (169)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −001/2	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$P\bar{4}b2$ No. 117 (170)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$: −110/2	(6) $\bar{h}kl$: −110/2	(7) $kh\bar{l}$: −110/2	(8) $\bar{k}\bar{h}\bar{l}$: −110/2

$P\bar{4}n2$ No. 118 (171)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$: −111/2	(6) $\bar{h}kl$: −111/2	(7) $kh\bar{l}$: −111/2	(8) $\bar{k}\bar{h}\bar{l}$: −111/2

$I\bar{4}m2$ No. 119 (172)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$:	(6) $\bar{h}kl$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$I\bar{4}c2$ No. 120 (173)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $h\bar{k}l$: −001/2	(6) $\bar{h}kl$: −001/2	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$I\bar{4}2m$ No. 121 (174)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $\bar{k}\bar{h}l$:	(8) khl:

$I\bar{4}2d$ No. 122 (175)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{k}h\bar{l}$:	(4) $k\bar{h}\bar{l}$:
(5) $\bar{h}k\bar{l}$: −203/4	(6) $h\bar{k}\bar{l}$: −203/4	(7) $\bar{k}\bar{h}l$: −021/4	(8) khl: −021/4

Point group: 4/*mmm* Tetragonal Laue group: 4/*mmm*

$P4/mmm$ No. 123 (176)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:

$P4/mcc$ No. 124 (177)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$: −001/2	(6) $h\bar{k}\bar{l}$: −001/2	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

$P4/nbm$ Origin 1 No. 125 (178)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:
(9) $\bar{h}\bar{k}\bar{l}$: −110/2	(10) $hk\bar{l}$: −110/2	(11) $\bar{k}h\bar{l}$: −110/2	(12) $k\bar{h}\bar{l}$: −110/2
(13) $h\bar{k}l$: −110/2	(14) $\bar{h}kl$: −110/2	(15) $\bar{k}\bar{h}l$: −110/2	(16) khl: −110/2

$P4/nbm$ Origin 2 No. 125 (179)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −100/2	(4) $\bar{k}hl$: −010/2
(5) $\bar{h}k\bar{l}$: −100/2	(6) $h\bar{k}\bar{l}$: −010/2	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$: −110/2

$P4/nnc$ Origin 1 No. 126 (180)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\bar{k}\bar{l}$:	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:
(9) $\bar{h}\bar{k}\bar{l}$: −111/2	(10) $hk\bar{l}$: −111/2	(11) $\bar{k}h\bar{l}$: −111/2	(12) $k\bar{h}\bar{l}$: −111/2
(13) $h\bar{k}l$: −111/2	(14) $\bar{h}kl$: −111/2	(15) $\bar{k}\bar{h}l$: −111/2	(16) khl: −111/2

$P4/nnc$ Origin 2 No. 126 (181)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −100/2	(4) $\bar{k}hl$: −010/2
(5) $\bar{h}k\bar{l}$: −101/2	(6) $h\bar{k}\bar{l}$: −011/2	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −111/2

$P4/mbm$ No. 127 (182)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\bar{k}\bar{l}$: −110/2	(7) $kh\bar{l}$: −110/2	(8) $\bar{k}\bar{h}\bar{l}$: −110/2

$P4/mnc$ No. 128 (183)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\bar{k}\bar{l}$: −111/2	(7) $kh\bar{l}$: −111/2	(8) $\bar{k}\bar{h}\bar{l}$: −111/2

$P4/nmm$ Origin 1 No. 129 (184)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −110/2	(4) $\bar{k}hl$: −110/2
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\bar{k}\bar{l}$: −110/2	(7) $kh\bar{l}$:	(8) $\bar{k}\bar{h}\bar{l}$:
(9) $\bar{h}\bar{k}\bar{l}$: −110/2	(10) $hk\bar{l}$: −110/2	(11) $\bar{k}h\bar{l}$:	(12) $k\bar{h}\bar{l}$:
(13) $h\bar{k}l$:	(14) $\bar{h}kl$:	(15) $\bar{k}\bar{h}l$: −110/2	(16) khl: −110/2

$P4/nmm$ Origin 2 No. 129 (185)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −100/2	(4) $\bar{k}hl$: −010/2
(5) $\bar{h}k\bar{l}$: −010/2	(6) $h\bar{k}\bar{l}$: −100/2	(7) $kh\bar{l}$: −110/2	(8) $\bar{k}\bar{h}\bar{l}$:

$P4/ncc$ Origin 1 No. 130 (186)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $k\bar{h}l$: −110/2	(4) $\bar{k}hl$: −110/2
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\bar{k}\bar{l}$: −111/2	(7) $kh\bar{l}$: −001/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2
(9) $\bar{h}\bar{k}\bar{l}$: −110/2	(10) $hk\bar{l}$: −110/2	(11) $\bar{k}h\bar{l}$:	(12) $k\bar{h}\bar{l}$:
(13) $h\bar{k}l$: −001/2	(14) $\bar{h}kl$: −001/2	(15) $\bar{k}\bar{h}l$: −111/2	(16) khl: −111/2

$P4/ncc$ Origin 2 No. 130 (187)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $k\bar{h}l$: −100/2	(4) $\bar{k}hl$: −010/2
(5) $\bar{h}k\bar{l}$: −011/2	(6) $h\bar{k}\bar{l}$: −101/2	(7) $kh\bar{l}$: −111/2	(8) $\bar{k}\bar{h}\bar{l}$: −001/2

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P4_2/mmc$ No. 131 (188)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $\bar{h}k\bar{l}$:	(6) $h\overline{kl}$:	(7) $kh\bar{l}$: −001/2	(8) $\overline{khl}$: −001/2

$P4_2/mcm$ No. 132 (189)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $\bar{h}k\bar{l}$: −001/2	(6) $h\overline{kl}$: −001/2	(7) $kh\bar{l}$:	(8) $\overline{khl}$:

$P4_2/nbc$ Origin 1 No. 133 (190)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$: −001/2	(6) $h\overline{kl}$: −001/2	(7) $kh\bar{l}$: −110/2	(8) $\overline{khl}$: −110/2
(9) $\overline{hkl}$: −111/2	(10) $hk\bar{l}$: −111/2	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$:
(13) $h\bar{k}l$: −110/2	(14) $\bar{h}kl$: −110/2	(15) $\overline{kh}l$: −001/2	(16) khl: −001/2

$P4_2/nbc$ Origin 2 No. 133 (191)

(1) hkl:	(2) $\overline{hk}l$: −110/2	(3) $k\bar{h}l$: −101/2	(4) $\bar{k}hl$: −011/2
(5) $\bar{h}k\bar{l}$: −100/2	(6) $h\overline{kl}$: −010/2	(7) $kh\bar{l}$: −001/2	(8) $\overline{khl}$: −111/2

$P4_2/nnm$ Origin 1 No. 134 (192)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$:	(6) $h\overline{kl}$:	(7) $kh\bar{l}$: −111/2	(8) $\overline{khl}$: −111/2
(9) $\overline{hkl}$: −111/2	(10) $hk\bar{l}$: −111/2	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$:
(13) $h\bar{k}l$: −111/2	(14) $\bar{h}kl$: −111/2	(15) $\overline{kh}l$:	(16) khl:

$P4_2/nnm$ Origin 2 No. 134 (193)

(1) hkl:	(2) $\overline{hk}l$: −110/2	(3) $k\bar{h}l$: −101/2	(4) $\bar{k}hl$: −011/2
(5) $\bar{h}k\bar{l}$: −101/2	(6) $h\overline{kl}$: −011/2	(7) $kh\bar{l}$:	(8) $\overline{khl}$: −110/2

$P4_2/mbc$ No. 135 (194)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −001/2	(4) $\bar{k}hl$: −001/2
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\overline{kl}$: −110/2	(7) $kh\bar{l}$: −111/2	(8) $\overline{khl}$: −111/2

$P4_2/mnm$ No. 136 (195)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\overline{kl}$: −111/2	(7) $kh\bar{l}$:	(8) $\overline{khl}$:

$P4_2/nmc$ Origin 1 No. 137 (196)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$: −111/2	(6) $h\overline{kl}$: −111/2	(7) $kh\bar{l}$:	(8) $\overline{khl}$:
(9) $\overline{hkl}$: −111/2	(10) $hk\bar{l}$: −111/2	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$:
(13) $h\bar{k}l$:	(14) $\bar{h}kl$:	(15) $\overline{kh}l$: −111/2	(16) khl: −111/2

$P4_2/nmc$ Origin 2 No. 137 (197)

(1) hkl:	(2) $\overline{hk}l$: −110/2	(3) $k\bar{h}l$: −101/2	(4) $\bar{k}hl$: −011/2
(5) $\bar{h}k\bar{l}$: −010/2	(6) $h\overline{kl}$: −100/2	(7) $kh\bar{l}$: −111/2	(8) $\overline{khl}$: −001/2

$P4_2/ncm$ Origin 1 No. 138 (198)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$: −111/2	(4) $\bar{k}hl$: −111/2
(5) $\bar{h}k\bar{l}$: −110/2	(6) $h\overline{kl}$: −110/2	(7) $kh\bar{l}$: −001/2	(8) $\overline{khl}$: −001/2
(9) $\overline{hkl}$: −111/2	(10) $hk\bar{l}$: −111/2	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$:
(13) $h\bar{k}l$: −001/2	(14) $\bar{h}kl$: −001/2	(15) $\overline{kh}l$: −110/2	(16) khl: −110/2

$P4_2/ncm$ Origin 2 No. 138 (199)

(1) hkl:	(2) $\overline{hk}l$: −110/2	(3) $k\bar{h}l$: −101/2	(4) $\bar{k}hl$: −011/2
(5) $\bar{h}k\bar{l}$: −011/2	(6) $h\overline{kl}$: −101/2	(7) $kh\bar{l}$: −110/2	(8) $\overline{khl}$:

$I4/mmm$ No. 139 (200)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$:	(6) $h\overline{kl}$:	(7) $kh\bar{l}$:	(8) $\overline{khl}$:

$I4/mcm$ No. 140 (201)

(1) hkl:	(2) $\overline{hk}l$:	(3) $k\bar{h}l$:	(4) $\bar{k}hl$:
(5) $\bar{h}k\bar{l}$: −001/2	(6) $h\overline{kl}$: −001/2	(7) $kh\bar{l}$: −001/2	(8) $\overline{khl}$: −001/2

$I4_1/amd$ Origin 1 No. 141 (202)

(1) hkl:	(2) $\overline{hk}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $\bar{h}k\bar{l}$: −203/4	(6) $h\overline{kl}$: −021/4	(7) $kh\bar{l}$: −111/2	(8) $\overline{khl}$:
(9) $\overline{hkl}$: −021/4	(10) $hk\bar{l}$: −203/4	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$: −111/2
(13) $h\bar{k}l$: −111/2	(14) $\bar{h}kl$:	(15) $\overline{kh}l$: −203/4	(16) khl: −021/4

$I4_1/amd$ Origin 2 No. 141 (203)

(1) hkl:	(2) $\overline{hk}l$: −101/2	(3) $k\bar{h}l$: −131/4	(4) $\bar{k}hl$: −113/4
(5) $\bar{h}k\bar{l}$: −101/2	(6) $h\overline{kl}$:	(7) $kh\bar{l}$: −131/4	(8) $\overline{khl}$: −113/4

$I4_1/acd$ Origin 1 No. 142 (204)

(1) hkl:	(2) $\overline{hk}l$: −111/2	(3) $k\bar{h}l$: −021/4	(4) $\bar{k}hl$: −203/4
(5) $\bar{h}k\bar{l}$: −201/4	(6) $h\overline{kl}$: −023/4	(7) $kh\bar{l}$: −110/2	(8) $\overline{khl}$: −001/2
(9) $\overline{hkl}$: −021/4	(10) $hk\bar{l}$: −203/4	(11) $\bar{k}h\bar{l}$:	(12) $k\overline{hl}$: −111/2
(13) $h\bar{k}l$: −110/2	(14) $\bar{h}kl$: −001/2	(15) $\overline{kh}l$: −201/4	(16) khl: −023/4

$I4_1/acd$ Origin 2 No. 142 (205)

(1) hkl:	(2) $\overline{hk}l$: −101/2	(3) $k\bar{h}l$: −131/4	(4) $\bar{k}hl$: −113/4
(5) $\bar{h}k\bar{l}$: −100/2	(6) $h\overline{kl}$: −001/2	(7) $kh\bar{l}$: −133/4	(8) $\overline{khl}$: −111/4

Point group: 3 Trigonal Laue group: $\bar{3}$

$P3$ No. 143 (206)

(1) hkl:	(2) kil:	(3) ihl:

$P3_1$ No. 144 (207)

(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3

$P3_2$ No. 145 (208)

(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3

$R3$ (hexagonal axes) No. 146 (209)

(1) hkl:	(2) kil:	(3) ihl:

$R3$ (rhombohedral axes) No. 146 (210)

(1) hkl:	(2) klh:	(3) lhk:

Point group: $\bar{3}$ Trigonal Laue group: $\bar{3}$

$P\bar{3}$ No. 147 (211)

(1) hkl:	(2) kil:	(3) ihl:

$R\bar{3}$ (hexagonal axes) No. 148 (212)

(1) hkl:	(2) kil:	(3) ihl:

$R\bar{3}$ (rhombohedral axes) No. 148 (213)

(1) hkl:	(2) klh:	(3) lhk:

Point group: 32 Trigonal Laue group: $\bar{3}m$

$P312$ No. 149 (214)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$:	(5) $\overline{hil}$:	(6) $\overline{ikl}$:

$P321$ No. 150 (215)

(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$:	(5) $hi\bar{l}$:	(6) $ik\bar{l}$:

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P3_112$ No. 151 (216)		
(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $\overline{khl}$: −002/3	(5) $\overline{hil}$: −001/3	(6) $\overline{ikl}$:
$P3_121$ No. 152 (217)		
(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $kh\bar{l}$:	(5) $hi\bar{l}$: −002/3	(6) $ik\bar{l}$: −001/3
$P3_212$ No. 153 (218)		
(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $\overline{khl}$: −001/3	(5) $\overline{hil}$: −002/3	(6) $\overline{ikl}$:
$P3_221$ No. 154 (219)		
(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $kh\bar{l}$:	(5) $hi\bar{l}$: −001/3	(6) $ik\bar{l}$: −002/3
$R32$ (hexagonal axes) No. 155 (220)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$:	(5) $hi\bar{l}$:	(6) $ik\bar{l}$:
$R32$ (rhombohedral axes) No. 155 (221)		
(1) hkl:	(2) klh:	(3) lhk:
(4) $\overline{khl}$:	(5) $\overline{hlk}$:	(6) $\overline{lkh}$:

Point group: 3*m* Trigonal Laue group: $\bar{3}m$

$P3m1$ No. 156 (222)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$:	(5) $\overline{hil}$:	(6) $\overline{ikl}$:
$P31m$ No. 157 (223)		
(1) hkl:	(2) kil:	(3) ihl:
(4) khl:	(5) hil:	(6) ikl:
$P3c1$ No. 158 (224)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$: −001/2	(5) $\overline{hil}$: −001/2	(6) $\overline{ikl}$: −001/2
$P31c$ No. 159 (225)		
(1) hkl:	(2) kil:	(3) ihl:
(4) khl: −001/2	(5) hil: −001/2	(6) ikl: −001/2
$R3m$ (hexagonal axes) No. 160 (226)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$:	(5) $\overline{hil}$:	(6) $\overline{ikl}$:
$R3m$ (rhombohedral axes) No. 160 (227)		
(1) hkl:	(2) klh:	(3) lhk:
(4) khl:	(5) hlk:	(6) lkh:
$R3c$ (hexagonal axes) No. 161 (228)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$: −001/2	(5) $\overline{hil}$: −001/2	(6) $\overline{ikl}$: −001/2
$R3c$ (rhombohedral axes) No. 161 (229)		
(1) hkl:	(2) klh:	(3) lhk:
(4) khl: −111/2	(5) hlk: −111/2	(6) lkh: −111/2

Point group: $\bar{3}m$ Trigonal Laue group: $\bar{3}m$

$P\bar{3}1m$ No. 162 (230)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$:	(5) $\overline{hil}$:	(6) $\overline{ikl}$:
$P\bar{3}1c$ No. 163 (231)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{khl}$: −001/2	(5) $\overline{hil}$: −001/2	(6) $\overline{ikl}$: −001/2
$P\bar{3}m1$ No. 164 (232)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$:	(5) $hi\bar{l}$:	(6) $ik\bar{l}$:
$P\bar{3}c1$ No. 165 (233)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$: −001/2	(5) $hi\bar{l}$: −001/2	(6) $ik\bar{l}$: −001/2
$R\bar{3}m$ (hexagonal axes) No. 166 (234)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$:	(5) $hi\bar{l}$:	(6) $ik\bar{l}$:
$R\bar{3}m$ (rhombohedral axes) No. 166 (235)		
(1) hkl:	(2) klh:	(3) lhk:
(4) $\overline{khl}$:	(5) $\overline{hlk}$:	(6) $\overline{lkh}$:
$R\bar{3}c$ (hexagonal axes) No. 167 (236)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $kh\bar{l}$: −001/2	(5) $hi\bar{l}$: −001/2	(6) $ik\bar{l}$: −001/2
$R\bar{3}c$ (rhombohedral axes) No. 168 (237)		
(1) hkl:	(2) klh:	(3) lhk:
(4) $\overline{khl}$: −111/2	(5) $\overline{hlk}$: −111/2	(6) $\overline{lkh}$: −111/2

Point group: 6 Hexagonal Laue group: 6/*m*

$P6$ No. 168 (238)		
(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:
$P6_1$ No. 169 (239)		
(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −005/6	(6) $\overline{ih}l$: −001/6
$P6_5$ No. 170 (240)		
(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/6	(6) $\overline{ih}l$: −005/6
$P6_2$ No. 171 (241)		
(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $\overline{hk}l$:	(5) $\overline{ki}l$: −002/3	(6) $\overline{ih}l$: −001/3
$P6_4$ No. 172 (242)		
(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $\overline{hk}l$:	(5) $\overline{ki}l$: −001/3	(6) $\overline{ih}l$: −002/3

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P6_3$ No. 173 (243)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/2	(6) $\overline{ih}l$: −001/2

Point group: $\bar{6}$ Hexagonal Laue group: 6/*m*

$P\bar{6}$ No. 174 (244)

(1) hkl:	(2) kil:	(3) ihl:
(4) $hk\bar{l}$:	(5) $ki\bar{l}$:	(6) $ih\bar{l}$:

Point group: 6/*m* Hexagonal Laue group: 6/*m*

$P6/m$ No. 175 (245)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:

$P6_3/m$ No. 176 (246)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/2	(6) $\overline{ih}l$: −001/2

Point group: 622 Hexagonal Laue group: 6/*mmm*

$P622$ No. 177 (247)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) $\overline{khl}$:	(11) $\overline{hil}$:	(12) $\overline{ikl}$:

$P6_122$ No. 178 (248)

(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −005/6	(6) $\overline{ih}l$: −001/6
(7) $kh\bar{l}$: −001/3	(8) $hi\bar{l}$:	(9) $ik\bar{l}$: −002/3
(10) $\overline{khl}$: −005/6	(11) $\overline{hil}$: −001/2	(12) $\overline{ikl}$: −001/6

$P6_522$ No. 179 (249)

(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/6	(6) $\overline{ih}l$: −005/6
(7) $kh\bar{l}$: −002/3	(8) $hi\bar{l}$:	(9) $ik\bar{l}$: −001/3
(10) $\overline{khl}$: −001/6	(11) $\overline{hil}$: −001/2	(12) $\overline{ikl}$: −005/6

$P6_222$ No. 180 (250)

(1) hkl:	(2) kil: −002/3	(3) ihl: −001/3
(4) $\overline{hk}l$:	(5) $\overline{ki}l$: −002/3	(6) $\overline{ih}l$: −001/3
(7) $kh\bar{l}$: −002/3	(8) $hi\bar{l}$:	(9) $ik\bar{l}$: −001/3
(10) $\overline{khl}$: −002/3	(11) $\overline{hil}$:	(12) $\overline{ikl}$: −001/3

$P6_422$ No. 181 (251)

(1) hkl:	(2) kil: −001/3	(3) ihl: −002/3
(4) $\overline{hk}l$:	(5) $\overline{ki}l$: −001/3	(6) $\overline{ih}l$: −002/3
(7) $kh\bar{l}$: −001/3	(8) $hi\bar{l}$:	(9) $ik\bar{l}$: −002/3
(10) $\overline{khl}$: −001/3	(11) $\overline{hil}$:	(12) $\overline{ikl}$: −002/3

$P6_322$ No. 182 (252)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/2	(6) $\overline{ih}l$: −001/2
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) $\overline{khl}$: −001/2	(11) $\overline{hil}$: −001/2	(12) $\overline{ikl}$: −001/2

Point group: 6*mm* Hexagonal Laue group: 6/*mmm*

$P6mm$ No. 183 (253)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:
(7) $\overline{kh}l$:	(8) $\overline{hi}l$:	(9) $\overline{ik}l$:
(10) khl:	(11) hil:	(12) ikl:

$P6cc$ No. 184 (254)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:
(7) $\overline{kh}l$: −001/2	(8) $\overline{hi}l$: −001/2	(9) $\overline{ik}l$: −001/2
(10) khl: −001/2	(11) hil: −001/2	(12) ikl: −001/2

$P6_3cm$ No. 185 (255)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/2	(6) $\overline{ih}l$: −001/2
(7) $\overline{kh}l$: −001/2	(8) $\overline{hi}l$: −001/2	(9) $\overline{ik}l$: −001/2
(10) khl:	(11) hil:	(12) ikl:

$P6_3mc$ No. 186 (256)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$: −001/2	(5) $\overline{ki}l$: −001/2	(6) $\overline{ih}l$: −001/2
(7) $\overline{kh}l$:	(8) $\overline{hi}l$:	(9) $\overline{ik}l$:
(10) khl: −001/2	(11) hil: −001/2	(12) ikl: −001/2

Point group: $\bar{6}m2$ Hexagonal Laue group: 6/*mmm*

$P\bar{6}m2$ No. 187 (257)

(1) hkl:	(2) kil:	(3) ihl:
(4) $hk\bar{l}$:	(5) $ki\bar{l}$:	(6) $ih\bar{l}$:
(7) $\overline{kh}l$:	(8) $\overline{hi}l$:	(9) $\overline{ik}l$:
(10) $\overline{khl}$:	(11) $\overline{hil}$:	(12) $\overline{ikl}$:

$P\bar{6}c2$ No. 188 (258)

(1) hkl:	(2) kil:	(3) ihl:
(4) $hk\bar{l}$: −001/2	(5) $ki\bar{l}$: −001/2	(6) $ih\bar{l}$: −001/2
(7) $\overline{kh}l$: −001/2	(8) $\overline{hi}l$: −001/2	(9) $\overline{ik}l$: −001/2
(10) $\overline{khl}$:	(11) $\overline{hil}$:	(12) $\overline{ikl}$:

$P\bar{6}2m$ No. 189 (259)

(1) hkl:	(2) kil:	(3) ihl:
(4) $hk\bar{l}$:	(5) $ki\bar{l}$:	(6) $ih\bar{l}$:
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) khl:	(11) hil:	(12) ikl:

$P\bar{6}2c$ No. 190 (260)

(1) hkl:	(2) kil:	(3) ihl:
(4) $hk\bar{l}$: −001/2	(5) $ki\bar{l}$: −001/2	(6) $ih\bar{l}$: −001/2
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) khl: −001/2	(11) hil: −001/2	(12) ikl: −001/2

Point group: 6/*mmm* Hexagonal Laue group: 6/*mmm*

$P6/mmm$ No. 191 (261)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\overline{hk}l$:	(5) $\overline{ki}l$:	(6) $\overline{ih}l$:
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) $\overline{khl}$:	(11) $\overline{hil}$:	(12) $\overline{ikl}$:

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

$P6/mcc$ No. 192 (262)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\bar{h}\bar{k}l$:	(5) $\bar{k}\bar{i}l$:	(6) $\bar{i}\bar{h}l$:
(7) $kh\bar{l}$: $-001/2$	(8) $hi\bar{l}$: $-001/2$	(9) $ik\bar{l}$: $-001/2$
(10) $\bar{k}\bar{h}\bar{l}$: $-001/2$	(11) $\bar{h}\bar{i}\bar{l}$: $-001/2$	(12) $\bar{i}\bar{k}\bar{l}$: $-001/2$

$P6_3/mcm$ No. 193 (263)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\bar{h}\bar{k}l$: $-001/2$	(5) $\bar{k}\bar{i}l$: $-001/2$	(6) $\bar{i}\bar{h}l$: $-001/2$
(7) $kh\bar{l}$: $-001/2$	(8) $hi\bar{l}$: $-001/2$	(9) $ik\bar{l}$: $-001/2$
(10) $\bar{k}\bar{h}\bar{l}$:	(11) $\bar{h}\bar{i}\bar{l}$:	(12) $\bar{i}\bar{k}\bar{l}$:

$P6_3/mmc$ No. 194 (264)

(1) hkl:	(2) kil:	(3) ihl:
(4) $\bar{h}\bar{k}l$: $-001/2$	(5) $\bar{k}\bar{i}l$: $-001/2$	(6) $\bar{i}\bar{h}l$: $-001/2$
(7) $kh\bar{l}$:	(8) $hi\bar{l}$:	(9) $ik\bar{l}$:
(10) $\bar{k}\bar{h}\bar{l}$: $-001/2$	(11) $\bar{h}\bar{i}\bar{l}$: $-001/2$	(12) $\bar{i}\bar{k}\bar{l}$: $-001/2$

Point group: 23 Cubic Laue group: $m\bar{3}$

$P23$ No. 195 (265)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$F23$ No. 196 (266)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$I23$ No. 197 (267)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$P2_13$ No. 198 (268)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-101/2$	(3) $\bar{h}k\bar{l}$: $-011/2$	(4) $h\bar{k}\bar{l}$: $-110/2$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-110/2$	(7) $\bar{k}l\bar{h}$: $-101/2$	(8) $k\bar{l}\bar{h}$: $-011/2$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-011/2$	(11) $\bar{l}h\bar{k}$: $-110/2$	(12) $l\bar{h}\bar{k}$: $-101/2$

$I2_13$ No. 199 (269)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-101/2$	(3) $\bar{h}k\bar{l}$: $-011/2$	(4) $h\bar{k}\bar{l}$: $-110/2$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-110/2$	(7) $\bar{k}l\bar{h}$: $-101/2$	(8) $k\bar{l}\bar{h}$: $-011/2$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-011/2$	(11) $\bar{l}h\bar{k}$: $-110/2$	(12) $l\bar{h}\bar{k}$: $-101/2$

Point group: $m\bar{3}$ Cubic Laue group: $m\bar{3}$

$Pm\bar{3}$ No. 200 (270)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$Pn\bar{3}$ Origin 1 No. 201 (271)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $\bar{h}\bar{k}\bar{l}$: $-111/2$	(14) $hk\bar{l}$: $-111/2$	(15) $h\bar{k}l$: $-111/2$	(16) $\bar{h}kl$: $-111/2$
(17) $\bar{k}\bar{l}\bar{h}$: $-111/2$	(18) $kl\bar{h}$: $-111/2$	(19) $k\bar{l}h$: $-111/2$	(20) $\bar{k}lh$: $-111/2$
(21) $\bar{l}\bar{h}\bar{k}$: $-111/2$	(22) $lh\bar{k}$: $-111/2$	(23) $l\bar{h}k$: $-111/2$	(24) $\bar{l}hk$: $-111/2$

$Pn\bar{3}$ Origin 2 No. 201 (272)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-110/2$	(3) $\bar{h}k\bar{l}$: $-101/2$	(4) $h\bar{k}\bar{l}$: $-011/2$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-011/2$	(7) $\bar{k}l\bar{h}$: $-110/2$	(8) $k\bar{l}\bar{h}$: $-101/2$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-101/2$	(11) $\bar{l}h\bar{k}$: $-011/2$	(12) $l\bar{h}\bar{k}$: $-110/2$

$Fm\bar{3}$ No. 202 (273)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$Fd\bar{3}$ Origin 1 No. 203 (274)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $\bar{h}\bar{k}\bar{l}$: $-111/4$	(14) $hk\bar{l}$: $-111/4$	(15) $h\bar{k}l$: $-111/4$	(16) $\bar{h}kl$: $-111/4$
(17) $\bar{k}\bar{l}\bar{h}$: $-111/4$	(18) $kl\bar{h}$: $-111/4$	(19) $k\bar{l}h$: $-111/4$	(20) $\bar{k}lh$: $-111/4$
(21) $\bar{l}\bar{h}\bar{k}$: $-111/4$	(22) $lh\bar{k}$: $-111/4$	(23) $l\bar{h}k$: $-111/4$	(24) $\bar{l}hk$: $-111/4$

$Fd\bar{3}$ Origin 2 No. 203 (275)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-110/4$	(3) $\bar{h}k\bar{l}$: $-101/4$	(4) $h\bar{k}\bar{l}$: $-011/4$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-011/4$	(7) $\bar{k}l\bar{h}$: $-110/4$	(8) $k\bar{l}\bar{h}$: $-101/4$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-101/4$	(11) $\bar{l}h\bar{k}$: $-011/4$	(12) $l\bar{h}\bar{k}$: $-110/4$

$Im\bar{3}$ No. 204 (276)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:

$Pa\bar{3}$ No. 205 (277)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-101/2$	(3) $\bar{h}k\bar{l}$: $-011/2$	(4) $h\bar{k}\bar{l}$: $-110/2$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-110/2$	(7) $\bar{k}l\bar{h}$: $-101/2$	(8) $k\bar{l}\bar{h}$: $-011/2$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-011/2$	(11) $\bar{l}h\bar{k}$: $-110/2$	(12) $l\bar{h}\bar{k}$: $-101/2$

$Ia\bar{3}$ No. 206 (278)

(1) hkl:	(2) $\bar{h}\bar{k}l$: $-101/2$	(3) $\bar{h}k\bar{l}$: $-011/2$	(4) $h\bar{k}\bar{l}$: $-110/2$
(5) klh:	(6) $\bar{k}\bar{l}h$: $-110/2$	(7) $\bar{k}l\bar{h}$: $-101/2$	(8) $k\bar{l}\bar{h}$: $-011/2$
(9) lhk:	(10) $\bar{l}\bar{h}k$: $-011/2$	(11) $\bar{l}h\bar{k}$: $-110/2$	(12) $l\bar{h}\bar{k}$: $-101/2$

Point group: 432 Cubic Laue group: $m\bar{3}m$

$P432$ No. 207 (279)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

$P4_232$ No. 208 (280)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$: $-111/2$	(14) $\bar{k}\bar{h}\bar{l}$: $-111/2$	(15) $\bar{k}hl$: $-111/2$	(16) $k\bar{h}l$: $-111/2$
(17) $h\bar{l}k$: $-111/2$	(18) $\bar{h}lk$: $-111/2$	(19) $\bar{h}\bar{l}\bar{k}$: $-111/2$	(20) $hl\bar{k}$: $-111/2$
(21) $\bar{l}kh$: $-111/2$	(22) $l\bar{k}h$: $-111/2$	(23) $lk\bar{h}$: $-111/2$	(24) $\bar{l}\bar{k}\bar{h}$: $-111/2$

$F432$ No. 209 (281)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

$F4_132$ No. 210 (282)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −011/2	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −101/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −101/2	(7) $\bar{k}l\bar{h}$: −011/2	(8) $k\bar{l}\bar{h}$: −110/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −110/2	(11) $\bar{l}\bar{h}k$: −101/2	(12) $l\bar{h}\bar{k}$: −011/2
(13) $kh\bar{l}$: −313/4	(14) $\bar{k}\bar{h}\bar{l}$: −111/4	(15) $\bar{k}hl$: −133/4	(16) $k\bar{h}l$: −331/4
(17) $h\bar{l}k$: −313/4	(18) $\bar{h}lk$: −331/4	(19) $\bar{h}\bar{l}\bar{k}$: −111/4	(20) $hl\bar{k}$: −133/4
(21) $\bar{l}kh$: −313/4	(22) $l\bar{k}h$: −133/4	(23) $lk\bar{h}$: −331/4	(24) $\bar{l}\bar{k}\bar{h}$: −111/4

$I432$ No. 211 (283)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

$P4_332$ No. 212 (284)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −110/2	(7) $\bar{k}l\bar{h}$: −101/2	(8) $k\bar{l}\bar{h}$: −011/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −011/2	(11) $\bar{l}\bar{h}k$: −110/2	(12) $l\bar{h}\bar{k}$: −101/2
(13) $kh\bar{l}$: −133/4	(14) $\bar{k}\bar{h}\bar{l}$: −111/4	(15) $\bar{k}hl$: −331/4	(16) $k\bar{h}l$: −313/4
(17) $h\bar{l}k$: −133/4	(18) $\bar{h}lk$: −313/4	(19) $\bar{h}\bar{l}\bar{k}$: −111/4	(20) $hl\bar{k}$: −331/4
(21) $\bar{l}kh$: −133/4	(22) $l\bar{k}h$: −331/4	(23) $lk\bar{h}$: −313/4	(24) $\bar{l}\bar{k}\bar{h}$: −111/4

$P4_132$ No. 213 (285)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −110/2	(7) $\bar{k}l\bar{h}$: −101/2	(8) $k\bar{l}\bar{h}$: −011/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −011/2	(11) $\bar{l}\bar{h}k$: −110/2	(12) $l\bar{h}\bar{k}$: −101/2
(13) $kh\bar{l}$: −311/4	(14) $\bar{k}\bar{h}\bar{l}$: −333/4	(15) $\bar{k}hl$: −113/4	(16) $k\bar{h}l$: −131/4
(17) $h\bar{l}k$: −311/4	(18) $\bar{h}lk$: −131/4	(19) $\bar{h}\bar{l}\bar{k}$: −333/4	(20) $hl\bar{k}$: −113/4
(21) $\bar{l}kh$: −311/4	(22) $l\bar{k}h$: −113/4	(23) $lk\bar{h}$: −131/4	(24) $\bar{l}\bar{k}\bar{h}$: −333/4

$I4_132$ No. 214 (286)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −110/2	(7) $\bar{k}l\bar{h}$: −101/2	(8) $k\bar{l}\bar{h}$: −011/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −011/2	(11) $\bar{l}\bar{h}k$: −110/2	(12) $l\bar{h}\bar{k}$: −101/2
(13) $kh\bar{l}$: −311/4	(14) $\bar{k}\bar{h}\bar{l}$: −333/4	(15) $\bar{k}hl$: −113/4	(16) $k\bar{h}l$: −131/4
(17) $h\bar{l}k$: −311/4	(18) $\bar{h}lk$: −131/4	(19) $\bar{h}\bar{l}\bar{k}$: −333/4	(20) $hl\bar{k}$: −113/4
(21) $\bar{l}kh$: −311/4	(22) $l\bar{k}h$: −113/4	(23) $lk\bar{h}$: −131/4	(24) $\bar{l}\bar{k}\bar{h}$: −333/4

Point group: $\bar{4}3m$ Cubic Laue group: $m\bar{3}m$

$P\bar{4}3m$ No. 215 (287)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) khl:	(14) $\bar{k}\bar{h}l$:	(15) $\bar{k}h\bar{l}$:	(16) $k\bar{h}\bar{l}$:
(17) hlk:	(18) $\bar{h}\bar{l}k$:	(19) $\bar{h}l\bar{k}$:	(20) $h\bar{l}\bar{k}$:
(21) lkh:	(22) $\bar{l}\bar{k}h$:	(23) $\bar{l}k\bar{h}$:	(24) $l\bar{k}\bar{h}$:

$F\bar{4}3m$ No. 216 (288)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) khl:	(14) $\bar{k}\bar{h}l$:	(15) $\bar{k}h\bar{l}$:	(16) $k\bar{h}\bar{l}$:
(17) hlk:	(18) $\bar{h}\bar{l}k$:	(19) $\bar{h}l\bar{k}$:	(20) $h\bar{l}\bar{k}$:
(21) lkh:	(22) $\bar{l}\bar{k}h$:	(23) $\bar{l}k\bar{h}$:	(24) $l\bar{k}\bar{h}$:

$I\bar{4}3m$ No. 217 (289)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) khl:	(14) $\bar{k}\bar{h}l$:	(15) $\bar{k}h\bar{l}$:	(16) $k\bar{h}\bar{l}$:
(17) hlk:	(18) $\bar{h}\bar{l}k$:	(19) $\bar{h}l\bar{k}$:	(20) $h\bar{l}\bar{k}$:
(21) lkh:	(22) $\bar{l}\bar{k}h$:	(23) $\bar{l}k\bar{h}$:	(24) $l\bar{k}\bar{h}$:

$P\bar{4}3n$ No. 218 (290)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) khl: −111/2	(14) $\bar{k}\bar{h}l$: −111/2	(15) $\bar{k}h\bar{l}$: −111/2	(16) $k\bar{h}\bar{l}$: −111/2
(17) hlk: −111/2	(18) $\bar{h}\bar{l}k$: −111/2	(19) $\bar{h}l\bar{k}$: −111/2	(20) $h\bar{l}\bar{k}$: −111/2
(21) lkh: −111/2	(22) $\bar{l}\bar{k}h$: −111/2	(23) $\bar{l}k\bar{h}$: −111/2	(24) $l\bar{k}\bar{h}$: −111/2

$F\bar{4}3c$ No. 219 (291)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) khl: −111/2	(14) $\bar{k}\bar{h}l$: −111/2	(15) $\bar{k}h\bar{l}$: −111/2	(16) $k\bar{h}\bar{l}$: −111/2
(17) hlk: −111/2	(18) $\bar{h}\bar{l}k$: −111/2	(19) $\bar{h}l\bar{k}$: −111/2	(20) $h\bar{l}\bar{k}$: −111/2
(21) lkh: −111/2	(22) $\bar{l}\bar{k}h$: −111/2	(23) $\bar{l}k\bar{h}$: −111/2	(24) $l\bar{k}\bar{h}$: −111/2

$I\bar{4}3d$ No. 220 (292)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −010/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −001/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −001/2	(7) $\bar{k}l\bar{h}$: −101/2	(8) $k\bar{l}\bar{h}$: −100/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −100/2	(11) $\bar{l}\bar{h}k$: −110/2	(12) $l\bar{h}\bar{k}$: −010/2
(13) khl: −111/4	(14) $\bar{k}\bar{h}l$: −311/4	(15) $\bar{k}h\bar{l}$: −313/4	(16) $k\bar{h}\bar{l}$: −113/4
(17) hlk: −111/4	(18) $\bar{h}\bar{l}k$: −113/4	(19) $\bar{h}l\bar{k}$: −133/4	(20) $h\bar{l}\bar{k}$: −131/4
(21) lkh: −111/4	(22) $\bar{l}\bar{k}h$: −131/4	(23) $\bar{l}k\bar{h}$: −331/4	(24) $l\bar{k}\bar{h}$: −311/4

Point group: $m\bar{3}m$ Cubic Laue group: $m\bar{3}m$

$Pm\bar{3}m$ No. 221 (293)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

$Pn\bar{3}n$ Origin 1 No. 222 (294)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}h\bar{k}$:	(11) $\bar{l}\bar{h}k$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:
(25) $\bar{h}\bar{k}\bar{l}$: −111/2	(26) $hk\bar{l}$: −111/2	(27) $h\bar{k}l$: −111/2	(28) $\bar{h}kl$: −111/2
(29) $\bar{k}\bar{l}\bar{h}$: −111/2	(30) $kl\bar{h}$: −111/2	(31) $k\bar{l}h$: −111/2	(32) $\bar{k}lh$: −111/2
(33) $\bar{l}\bar{h}\bar{k}$: −111/2	(34) $l\bar{h}k$: −111/2	(35) $lh\bar{k}$: −111/2	(36) $\bar{l}hk$: −111/2
(37) $\bar{k}\bar{h}l$: −111/2	(38) khl: −111/2	(39) $k\bar{h}\bar{l}$: −111/2	(40) $\bar{k}h\bar{l}$: −111/2
(41) $\bar{h}l\bar{k}$: −111/2	(42) $h\bar{l}\bar{k}$: −111/2	(43) hlk: −111/2	(44) $\bar{h}\bar{l}k$: −111/2
(45) $l\bar{k}\bar{h}$: −111/2	(46) $\bar{l}k\bar{h}$: −111/2	(47) $\bar{l}\bar{k}h$: −111/2	(48) lkh: −111/2

$Pn\bar{3}n$ Origin 2 No. 222 (295)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −101/2	(4) $h\bar{k}\bar{l}$: −011/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −011/2	(7) $\bar{k}l\bar{h}$: −110/2	(8) $k\bar{l}\bar{h}$: −101/2
(9) lhk:	(10) $\bar{l}h\bar{k}$: −101/2	(11) $\bar{l}\bar{h}k$: −011/2	(12) $l\bar{h}\bar{k}$: −110/2
(13) $kh\bar{l}$: −001/2	(14) $\bar{k}\bar{h}\bar{l}$: −111/2	(15) $\bar{k}hl$: −010/2	(16) $k\bar{h}l$: −100/2

Table A1.4.4.1. *Crystallographic space groups in reciprocal space* (*cont.*)

(17) $h\bar{l}k$: −001/2	(18) $\bar{h}lk$: −100/2	(19) $\bar{h}\bar{l}\bar{k}$: −111/2	(20) $hl\bar{k}$: −010/2
(21) $\bar{l}kh$: −001/2	(22) $l\bar{k}h$: −010/2	(23) $lk\bar{h}$: −100/2	(24) $\bar{l}\bar{k}\bar{h}$: −111/2

Pm$\bar{3}$*n* No. 223 (296)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$: −111/2	(14) $\bar{k}\bar{h}\bar{l}$: −111/2	(15) $\bar{k}hl$: −111/2	(16) $k\bar{h}l$: −111/2
(17) $h\bar{l}k$: −111/2	(18) $\bar{h}lk$: −111/2	(19) $\bar{h}\bar{l}\bar{k}$: −111/2	(20) $hl\bar{k}$: −111/2
(21) $\bar{l}kh$: −111/2	(22) $l\bar{k}h$: −111/2	(23) $lk\bar{h}$: −111/2	(24) $\bar{l}\bar{k}\bar{h}$: −111/2

Pn$\bar{3}$*m* Origin 1 No. 224 (297)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$: −111/2	(14) $\bar{k}\bar{h}\bar{l}$: −111/2	(15) $\bar{k}hl$: −111/2	(16) $k\bar{h}l$: −111/2
(17) $h\bar{l}k$: −111/2	(18) $\bar{h}lk$: −111/2	(19) $\bar{h}\bar{l}\bar{k}$: −111/2	(20) $hl\bar{k}$: −111/2
(21) $\bar{l}kh$: −111/2	(22) $l\bar{k}h$: −111/2	(23) $lk\bar{h}$: −111/2	(24) $\bar{l}\bar{k}\bar{h}$: −111/2
(25) $\bar{h}\bar{k}\bar{l}$: −111/2	(26) $hk\bar{l}$: −111/2	(27) $h\bar{k}l$: −111/2	(28) $\bar{h}kl$: −111/2
(29) $\bar{k}\bar{l}\bar{h}$: −111/2	(30) $kl\bar{h}$: −111/2	(31) $k\bar{l}h$: −111/2	(32) $\bar{k}lh$: −111/2
(33) $\bar{l}\bar{h}\bar{k}$: −111/2	(34) $lh\bar{k}$: −111/2	(35) $l\bar{h}k$: −111/2	(36) $\bar{l}hk$: −111/2
(37) $\bar{k}\bar{h}l$:	(38) khl:	(39) $k\bar{h}\bar{l}$:	(40) $\bar{k}h\bar{l}$:
(41) $\bar{h}l\bar{k}$:	(42) $h\bar{l}\bar{k}$:	(43) hlk:	(44) $\bar{h}\bar{l}k$:
(45) $l\bar{k}\bar{h}$:	(46) $\bar{l}k\bar{h}$:	(47) $\bar{l}\bar{k}h$:	(48) lkh:

Pn$\bar{3}$*m* Origin 2 No. 224 (298)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −110/2	(3) $\bar{h}k\bar{l}$: −101/2	(4) $h\bar{k}\bar{l}$: −011/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −011/2	(7) $\bar{k}l\bar{h}$: −110/2	(8) $k\bar{l}\bar{h}$: −101/2
(9) lhk:	(10) $\bar{l}\bar{h}k$: −101/2	(11) $\bar{l}h\bar{k}$: −011/2	(12) $l\bar{h}\bar{k}$: −110/2
(13) $kh\bar{l}$: −110/2	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$: −101/2	(16) $k\bar{h}l$: −011/2
(17) $h\bar{l}k$: −110/2	(18) $\bar{h}lk$: −011/2	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$: −101/2
(21) $\bar{l}kh$: −110/2	(22) $l\bar{k}h$: −101/2	(23) $lk\bar{h}$: −011/2	(24) $\bar{l}\bar{k}\bar{h}$:

Fm$\bar{3}$*m* No. 225 (299)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

Fm$\bar{3}$*c* No. 226 (300)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$: −111/2	(14) $\bar{k}\bar{h}\bar{l}$: −111/2	(15) $\bar{k}hl$: −111/2	(16) $k\bar{h}l$: −111/2
(17) $h\bar{l}k$: −111/2	(18) $\bar{h}lk$: −111/2	(19) $\bar{h}\bar{l}\bar{k}$: −111/2	(20) $hl\bar{k}$: −111/2
(21) $\bar{l}kh$: −111/2	(22) $l\bar{k}h$: −111/2	(23) $lk\bar{h}$: −111/2	(24) $\bar{l}\bar{k}\bar{h}$: −111/2

Fd$\bar{3}$*m* Origin 1 No. 227 (301)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −011/2	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −101/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −101/2	(7) $\bar{k}l\bar{h}$: −011/2	(8) $k\bar{l}\bar{h}$: −110/2
(9) lhk:	(10) $\bar{l}\bar{h}k$: −110/2	(11) $\bar{l}h\bar{k}$: −101/2	(12) $l\bar{h}\bar{k}$: −011/2
(13) $kh\bar{l}$: −313/4	(14) $\bar{k}\bar{h}\bar{l}$: −111/4	(15) $\bar{k}hl$: −133/4	(16) $k\bar{h}l$: −331/4
(17) $h\bar{l}k$: −313/4	(18) $\bar{h}lk$: −331/4	(19) $\bar{h}\bar{l}\bar{k}$: −111/4	(20) $hl\bar{k}$: −133/4
(21) $\bar{l}kh$: −313/4	(22) $l\bar{k}h$: −133/4	(23) $lk\bar{h}$: −331/4	(24) $\bar{l}\bar{k}\bar{h}$: −111/4
(25) $\bar{h}\bar{k}\bar{l}$: −111/4	(26) $hk\bar{l}$: −133/4	(27) $h\bar{k}l$: −331/4	(28) $\bar{h}kl$: −313/4
(29) $\bar{k}\bar{l}\bar{h}$: −111/4	(30) $kl\bar{h}$: −313/4	(31) $k\bar{l}h$: −133/4	(32) $\bar{k}lh$: −331/4
(33) $\bar{l}\bar{h}\bar{k}$: −111/4	(34) $lh\bar{k}$: −331/4	(35) $l\bar{h}k$: −313/4	(36) $\bar{l}hk$: −133/4
(37) $\bar{k}\bar{h}l$: −101/2	(38) khl:	(39) $k\bar{h}\bar{l}$: −011/2	(40) $\bar{k}h\bar{l}$: −110/2
(41) $\bar{h}l\bar{k}$: −101/2	(42) $h\bar{l}\bar{k}$: −110/2	(43) hlk:	(44) $\bar{h}\bar{l}k$: −011/2
(45) $l\bar{k}\bar{h}$: −101/2	(46) $\bar{l}k\bar{h}$: −011/2	(47) $\bar{l}\bar{k}h$: −110/2	(48) lkh:

Fd$\bar{3}$*m* Origin 2 No. 227 (302)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −312/4	(3) $\bar{h}k\bar{l}$: −123/4	(4) $h\bar{k}\bar{l}$: −231/4
(5) klh:	(6) $\bar{k}\bar{l}h$: −231/4	(7) $\bar{k}l\bar{h}$: −312/4	(8) $k\bar{l}\bar{h}$: −123/4
(9) lhk:	(10) $\bar{l}\bar{h}k$: −123/4	(11) $\bar{l}h\bar{k}$: −231/4	(12) $l\bar{h}\bar{k}$: −312/4
(13) $kh\bar{l}$: −312/4	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$: −123/4	(16) $k\bar{h}l$: −231/4
(17) $h\bar{l}k$: −312/4	(18) $\bar{h}lk$: −231/4	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$: −123/4
(21) $\bar{l}kh$: −312/4	(22) $l\bar{k}h$: −123/4	(23) $lk\bar{h}$: −231/4	(24) $\bar{l}\bar{k}\bar{h}$:

Fd$\bar{3}$*c* Origin 1 No. 228 (303)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −011/2	(3) $\bar{h}k\bar{l}$: −110/2	(4) $h\bar{k}\bar{l}$: −101/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −101/2	(7) $\bar{k}l\bar{h}$: −011/2	(8) $k\bar{l}\bar{h}$: −110/2
(9) lhk:	(10) $\bar{l}\bar{h}k$: −110/2	(11) $\bar{l}h\bar{k}$: −101/2	(12) $l\bar{h}\bar{k}$: −011/2
(13) $kh\bar{l}$: −313/4	(14) $\bar{k}\bar{h}\bar{l}$: −111/4	(15) $\bar{k}hl$: −133/4	(16) $k\bar{h}l$: −331/4
(17) $h\bar{l}k$: −313/4	(18) $\bar{h}lk$: −331/4	(19) $\bar{h}\bar{l}\bar{k}$: −111/4	(20) $hl\bar{k}$: −133/4
(21) $\bar{l}kh$: −313/4	(22) $l\bar{k}h$: −133/4	(23) $lk\bar{h}$: −331/4	(24) $\bar{l}\bar{k}\bar{h}$: −111/4
(25) $\bar{h}\bar{k}\bar{l}$: −333/4	(26) $hk\bar{l}$: −311/4	(27) $h\bar{k}l$: −113/4	(28) $\bar{h}kl$: −131/4
(29) $\bar{k}\bar{l}\bar{h}$: −333/4	(30) $kl\bar{h}$: −131/4	(31) $k\bar{l}h$: −311/4	(32) $\bar{k}lh$: −113/4
(33) $\bar{l}\bar{h}\bar{k}$: −333/4	(34) $lh\bar{k}$: −113/4	(35) $l\bar{h}k$: −131/4	(36) $\bar{l}hk$: −311/4
(37) $\bar{k}\bar{h}l$: −010/2	(38) khl: −111/2	(39) $k\bar{h}\bar{l}$: −100/2	(40) $\bar{k}h\bar{l}$: −001/2
(41) $\bar{h}l\bar{k}$: −010/2	(42) $h\bar{l}\bar{k}$: −001/2	(43) hlk: −111/2	(44) $\bar{h}\bar{l}k$: −100/2
(45) $l\bar{k}\bar{h}$: −010/2	(46) $\bar{l}k\bar{h}$: −100/2	(47) $\bar{l}\bar{k}h$: −001/2	(48) lkh: −111/2

Fd$\bar{3}$*c* Origin 2 No. 228 (304)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −132/4	(3) $\bar{h}k\bar{l}$: −321/4	(4) $h\bar{k}\bar{l}$: −213/4
(5) klh:	(6) $\bar{k}\bar{l}h$: −213/4	(7) $\bar{k}l\bar{h}$: −132/4	(8) $k\bar{l}\bar{h}$: −321/4
(9) lhk:	(10) $\bar{l}\bar{h}k$: −321/4	(11) $\bar{l}h\bar{k}$: −213/4	(12) $l\bar{h}\bar{k}$: −132/4
(13) $kh\bar{l}$: −310/4	(14) $\bar{k}\bar{h}\bar{l}$: −111/2	(15) $\bar{k}hl$: −103/4	(16) $k\bar{h}l$: −031/4
(17) $h\bar{l}k$: −310/4	(18) $\bar{h}lk$: −031/4	(19) $\bar{h}\bar{l}\bar{k}$: −111/2	(20) $hl\bar{k}$: −103/4
(21) $\bar{l}kh$: −310/4	(22) $l\bar{k}h$: −103/4	(23) $lk\bar{h}$: −031/4	(24) $\bar{l}\bar{k}\bar{h}$: −111/2

Im$\bar{3}$*m* No. 229 (305)

(1) hkl:	(2) $\bar{h}\bar{k}l$:	(3) $\bar{h}k\bar{l}$:	(4) $h\bar{k}\bar{l}$:
(5) klh:	(6) $\bar{k}\bar{l}h$:	(7) $\bar{k}l\bar{h}$:	(8) $k\bar{l}\bar{h}$:
(9) lhk:	(10) $\bar{l}\bar{h}k$:	(11) $\bar{l}h\bar{k}$:	(12) $l\bar{h}\bar{k}$:
(13) $kh\bar{l}$:	(14) $\bar{k}\bar{h}\bar{l}$:	(15) $\bar{k}hl$:	(16) $k\bar{h}l$:
(17) $h\bar{l}k$:	(18) $\bar{h}lk$:	(19) $\bar{h}\bar{l}\bar{k}$:	(20) $hl\bar{k}$:
(21) $\bar{l}kh$:	(22) $l\bar{k}h$:	(23) $lk\bar{h}$:	(24) $\bar{l}\bar{k}\bar{h}$:

Ia$\bar{3}$*d* No. 230 (306)

(1) hkl:	(2) $\bar{h}\bar{k}l$: −101/2	(3) $\bar{h}k\bar{l}$: −011/2	(4) $h\bar{k}\bar{l}$: −110/2
(5) klh:	(6) $\bar{k}\bar{l}h$: −110/2	(7) $\bar{k}l\bar{h}$: −101/2	(8) $k\bar{l}\bar{h}$: −011/2
(9) lhk:	(10) $\bar{l}\bar{h}k$: −011/2	(11) $\bar{l}h\bar{k}$: −110/2	(12) $l\bar{h}\bar{k}$: −101/2
(13) $kh\bar{l}$: −311/4	(14) $\bar{k}\bar{h}\bar{l}$: −333/4	(15) $\bar{k}hl$: −113/4	(16) $k\bar{h}l$: −131/4
(17) $h\bar{l}k$: −311/4	(18) $\bar{h}lk$: −131/4	(19) $\bar{h}\bar{l}\bar{k}$: −333/4	(20) $hl\bar{k}$: −113/4
(21) $\bar{l}kh$: −311/4	(22) $l\bar{k}h$: −113/4	(23) $lk\bar{h}$: −131/4	(24) $\bar{l}\bar{k}\bar{h}$: −333/4

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