Chapter 6
Symmetry Analysis for Crystals and the Use of the International Tables

6.1 Symmetry Analysis

A crystal may be defined as a solid composed of atoms arranged on a regular three-dimensional lattice and such periodicity in the atomic distribution features their structure. The geometry of atomic distributions in crystals is known to be characterized by the repetition, such as lattice translation (see Chap. 2). In addition to lattice translations, we find reflection and rotation. In these cases, an object is brought into coincidence with itself by reflection in a certain plane; rotation upon around a certain axis; or reflection in a certain plane. The repetition of a pattern by specific rules characterizes all symmetry operations and their fundamental points are given below.

If a symmetry operation leaves a locus, such as a point, a line, or a plane unchanged (i.e., same atomic position), this locus is referred to as the symmetry element. For any operation excluding lattice translation for space group, the symmetry operation belongs to one of four cases: inversion (i) expressed by a change from (x, y, z) to $(-x, -y, -z)$; rotatory-inversion ($\bar{n}$); reflection (m: a mirror plane) expressed by a change from (x, y, z) to $(-x, y, z)$; and rotation (n, a rotation axis) expressed by a change $(360°/n)$ about an axis. In crystals, we may conclude that only one-, two-, three-, four-, and sixfold rotation axes can be accepted. Of course, the symmetry operations may be linked with one another. The symmetry operation called inversion relates a pairs of objects which are equidistant from and on opposite sides of a central point (called inversion center). That is, only a single point remains unchanged. Whereas, rotatory-inversion is one of the compound symmetry operations and it is frequently called roto-inversion. This operation is produced by the combination of a rotation of $(360°/n)$ around a certain axis followed by inversion through a point on the axis as a symmetry center.

As shown in Fig. 6.1, the rotatory-inversion operation provides five cases denoted by symbols $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, and $\bar{6}$. However, the following three points are noteworthy. (1) Since the rotatory-inversion operation of $\bar{1}$ is a rotation of 360° followed by inversion through a point on the onefold roto-inversion axis, it is identical to inversion (i), simply called center of symmetry or inversion center. (2) The rotatory-inversion operation of $\bar{2}$ is represented by rotation through an angle of 180° followed by inversion to take one point into an equivalent one. However, these two points are

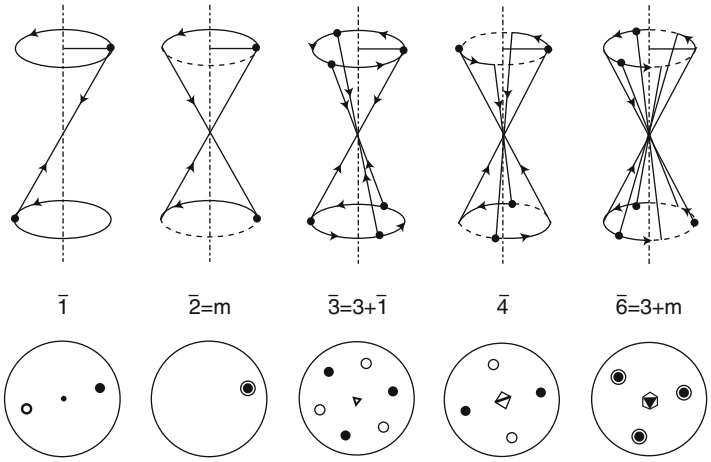


Fig. 6.1 Examples of rotatory-inversion operation

also related to one another by reflection in a plane normal to the axis, so that the rotatory-inversion of $\bar{2}$ is identical to a mirror reflection (m). (3) As easily seen in Fig. 6.1, successive applications of the rotation-inversion operation of $\bar{3}$ alter a point into altogether six equivalent positions. This variation can be reproduced by combining operations with a threefold rotation axis and inversion (i). Similarly, the rotation-inversion operation of $\bar{6}$ is also represented by combining operations with a threefold rotation axis and a twofold roto-inversion axis, or mirror plane perpendicular to the axis. These three points suggest that the rotatory-inversion operations except for $\bar{4}$ result in no new operation, so that $\bar{1}$, $\bar{2}$, $\bar{3}$, and $\bar{6}$ are not included in the independent symmetry operations.

For convenience, some additional details are given for understanding the rotatory-inversion operation of $\bar{4}$, using two different cases as an example. In Fig. 6.2a, we easily find the results obtained by symmetry operations of fourfold rotation and inversion, because successive operations about the fourfold axis move a point from 1 to 2, 3, 4, and back to 1. On the other hand, the inversion center alters it from each of those positions to 7, 8, 5, and 6, respectively. This combination of symmetry operations results in a mirror plane normal to the axis. In this case, two individual symmetry operations are found to be linked which are themselves symmetry operations. Whereas, in Fig. 6.2b illustrating the results obtained by symmetry operation of fourfold rotation about an axis followed by inversion through a point on its axis. Successive applications of these operations move a point at 1 to 2, 3, 4, and back to 1. In this case, we can find neither the inversion center nor the fourfold rotation axis (see auxiliary points denoted by open circles in Fig. 6.2b. Namely, two symmetry operations in this case are made in sequence as a single matter referred to as a new symmetry operation, which is called compound symmetry operation.

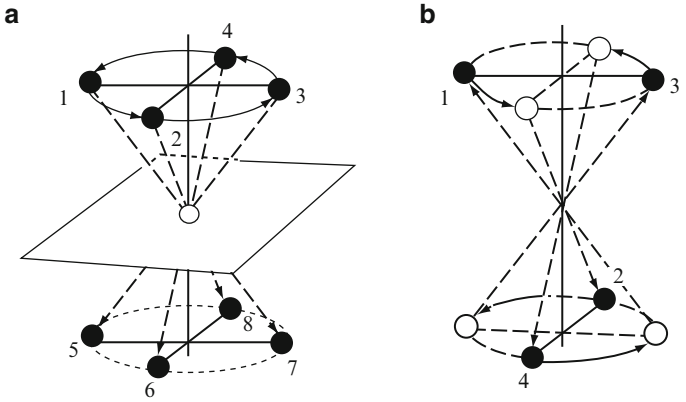


Fig. 6.2 Applications of the fourfold rotation and inversion. (**a**) Combination of independent symmetry operation, (**b**) Compound operation (roto-inversion)

In conclusion, the independent symmetry operations for discussing the symmetry of the three-dimensional atomic arrangement are eight: inversion (i), reflection (m), rotation (1, 2, 3, 4, 6), and rotatory-inversion of $\bar{4}$. This means that the whole periodic array observed in crystals can be covered by repeating the parallel translation (translational operation) of the structure derived from these eight kinds of symmetry element. In other words, as already mentioned in Chap. 2, there are seven crystal systems for classification, which consist of 14 kinds of Bravais lattices and a crystal is known to be classified into 32 point groups on the basis of eight kinds of symmetry element. In addition, when it is extended to include space groups, by adding point groups, Bravais lattices, screw axis, and glide reflection plane, it will be classified into 230 in total. For this analysis, we have to include two compound symmetry operations; rotation and translation (screw axis) and reflection and translation (glide plane). A brief description for screw axes and glide reflection planes is given below.

The symmetry operation of the so-called "screw rotation" consists of a rotation of $360°/n$ where n is 2, 3, 4, and 6 and a translation by a vector parallel to the axis. The screw axis is expressed by n_m and its operation is to translate by (m/n) times the length of a unit lattice vector along the direction of a rotation axis every one operation with respect to n-axis of rotation. All of the screw rotation axes are shown in Fig. 6.3 (see also Question 6.1). Although the direction of rotation itself is not so important in the screw rotation, the definition is illustrated in Fig. 6.4 using a right-handed axial system as an example. This case shows an operation which is a rotation around a c-axis from the a-axis toward the b-axis by an angle ϕ followed by a positive translation along a c-axis, called the motion of a right-handed screw.

The compound symmetry operation of a glide reflection consists of a reflection and a translation by the vector $\boldsymbol{q}_g$ parallel to the plane of reflection. For convenience, Fig. 6.5 shows a comparison of the operation of a glide plane with that of a mirror plane on a point lying off the planes.

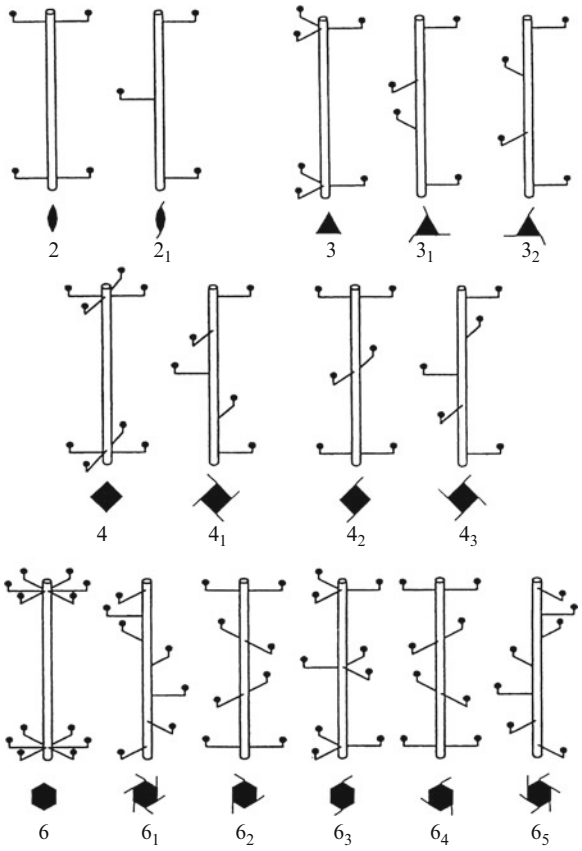


Fig. 6.3 Examples of possible screw axes

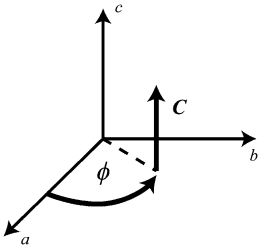


Fig. 6.4 A right-handed screw system

The description of this symmetry element may also be simplified by reference to the unit lattice vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$. For example, with respect to a-glide plane perpendicular to the b-direction, the reflection operation is made through the glide plane and then displaced by the vector, corresponding to one-half of a lattice translation $\left(\frac{1}{2}\boldsymbol{a}\right)$, parallel to the glide plane. Similarly, we may obtain b- and c-glide planes perpendicular to one of the other directions. There is also a diagonal glide plane n by

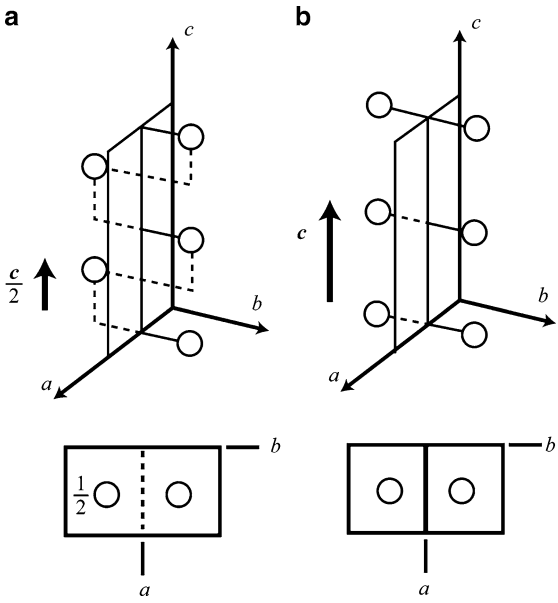


Fig. 6.5 Comparison of the operation of (**a**) a glide plane and (**b**) a mirror plane

translation of the diagonal direction. That is, the n-glide plane, if it is perpendicular to c, gives a glide component of $\left(\frac{1}{2}\boldsymbol{a} + \frac{1}{2}\boldsymbol{b}\right)$. Furthermore, we have one additional case; the diamond glide plane denoted by d which can be featured by one quarter $(1/4)$ of a lattice translation along the line parallel to the body-centered direction. Then, there are five kinds of glide reflection planes in all.

As mentioned previously, all crystal structures can be classified into seven crystal systems using parameters of three vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ (or those lengths a, b, and c) and the interaxial angles between them, α, β, and γ. The relationships between crystal systems and symmetry elements are summarized in Table 6.1.

The atomic distribution in crystals is characterized by its periodicity in a regular three-dimensional lattice and it is known to be classified into 32 point groups using eight symmetry elements (see Fig. 2.1). In addition, the periodicity in regular three-dimensional lattice can be analyzed by the concept of symmetry. Particularly, if we use eight kinds of symmetry element; "reflection (m)," "rotation (1, 2, 3, 4 and 6)," "inversion (i)," and "rotatory-inversion ($\bar{4}$)" together with eleven "screw axes" and five "glide planes," all the possible geometric arrangement of atoms in three-dimensional lattice space can be classified into 230 in all, called "space groups." This implies that the number of geometric arrangements with periodicity is limited in three-dimensional lattice space. In other words, any crystal can be described only by one of the 230 space groups. In addition, the real crystal structures are not evenly distributed over these 230 space groups. It is rather unevenly distributed, so that there are many space groups that do not represent any real crystal structure. The relationships of crystal systems with point group and space groups are summarized in Table 6.2.

Table 6.1 Seven crystal systems, symmetry elements, and relevant data

Crystal systems	Subunit	Minimum symmetry elements	Point groups	Number of rotation axes 2346	Number of mirror plane
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	None	$1, \bar{1}$	0000	0
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \beta \neq 90^\circ$	One diad axis or mirror plane	$2, m$, 2/m	1000	1
Orthorhombic	$a \neq b \neq c$	Three orthogonal diad or inverse diad axis	$222, mm2,$ mmm	3000	3
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	One tetrad or inverse tetrad axis	$4, \bar{4}, 4/m,$ $422, 4mm,$ $\bar{4}2m, 4/mmm$	4010	5
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Form triad axes	$23, m3, 432,$ $\bar{4}3m\ m3m$	6430	9
Trigonal	$a = b \neq c$ $\alpha = \beta = 90^\circ\ \gamma = 120^\circ$ or $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	One triad or inverse triad axis	$3, \bar{3}, 32, 3m, \bar{3}m$	3100	3
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	One hexad or inverse hexad axis	$6, \bar{6}, 6/m622,$ $6mm, \bar{6}m2,$ $6/mmm$	6001	7

6.2 International Tables

It is not necessary to know all (230) the space groups individually, because we can easily get many of the most important information of the space groups from "International Tables for Crystallography Vol. A, Fifth Edition (2002)" published by the International Union of Crystallography (referred to as IUCr). Although two methods, Schönflies symbols and Hermann–Mauguin symbols have been used for describing the 32 point groups (see Question 6.2), the IUCr suggests the use of Hermann–Mauguin symbols. Note that Schönflies symbols are widely used in respect to spectroscopy, especially of organic molecules. This handbook is quite useful for determining or interpreting the structure of crystals of interest. Although the contents cover only 24 space groups frequently found in real crystals, a textbook is also available for beginners titled on Brief Teaching Edition of Volume A Space-group Symmetry, International Tables for Crystallography, Fifth Revised Edition, edited by T. Hahn, Kluwer Academic Publishers, Dordrecht, and Holland (2002). International Tables for Crystallography (often referred to as International Tables) provides the following information:

(1) Short space group symbol, Schönflies symbol, point group, crystal system, number of the space group, full space group symbol, and Patterson symmetry symbol.

Table 6.2 Crystal systems and relations to point groups and space groups

Crystal system	Point	Space groups
Triclinic	1	$P1$
	$\bar{1}$	$P\bar{1}$
Monoclinic	2	$P2$, $P2_1$, $C2$
	m	*Pm, Pc, Cm, Cc*
	2/m	*P2/m* , $P2_1/m$, *C2/m*, *P2/c*, $P2_1/c$, *C2/c*
Orthorhombic	222	*P222*, $P222_1$, $P2_12_12$, $P2_12_12_1$, $C222_1$, *C222*, *F222*, *I222*, $I2_12_12_1$
	mm2	*Pmm2*, $Pmc2_1$, *Pcc2*, $Pma2_1$, $Pca2_1$, $Pnc2_1$, $Pmn2_1$, *Pba2*, $Pna2_1$, *Pnn2*, *Cmm2*, $Cmc2_1$, *Ccc2*, *Amm2*, *Abm2*, *Ama2*, *Aba2*, *Fmm2*, *Fdd2*, *Imm2*, *Iba2*, *Ima2*, *Aba2*, *Fmm2*, *Fdd2*, *Imm2*, *Iba2*, *Ima2*
	mmm	*Pmmm, Pnnn, Pccm, Pban, Pmma, Pnna, Pmna, Pcca, Pbam, Pccn, Pbcm, Pnnm, Pmmn, Pbcn, Pbca, Pnma, Cmcm, Cmca, Cmmm, Cccm, Cmma, Ccca, Fmmm, Fddd, Immm, Ibam, Ibca, Imma*
Tetragonal	4	$P4$, $P4_1$, $P4_2$, $P4_3$, $I4$, $I4_1$
	$\bar{4}$	$P\bar{4}$, $I\bar{4}$
	$4/m$	$P4/m$, $P4_2/m$, $P4/n$, $P4_2/n$, $I4/m$, $I4_1/a$
	422	$P422$, $P42_12$, $P4_122$, $P4_12_12$, $P4_222$, $P4_22_12$ $P4_322$, $P4_32_12$, $I422$, $I4_122$
	4mm	*P4mm*, *P4bm*, $P4_2cm$, $P4_2nm$, *P4cc*, *P4nc*, $P4_2mc$, $P4_2bc$, *I4mn*, *I4cm*, $I4_1md$, *I4cd*
	$\bar{4}2m$	$P\bar{4}2m$, $P\bar{4}2c$, $P\bar{4}2_1m$, $P\bar{4}2_1c$, $P\bar{4}m2$, $P\bar{4}c2$, $P\bar{4}b2$, $P\bar{4}n2$, $I\bar{4}m2$, $I\bar{4}c2$, $I\bar{4}2m$, $I\bar{4}2d$
	4/mmm	$P4/mmm$, $P4/mcc$, $P4/nbm$, $P4/nnc$, $P4/mbm$, $P4/mnc$, $P4/nmm$, $P4/ncc$, $P4_2/mmc$, $P4_2/mcm$, $P4_2/nbc$, $P4_2/nnm$, $P4_2/mbc$, $P4_2/mnm$, $P4_2/nmc$, $P4_2/ncm$, $I4/mmm$, $I4/mcm$, $I4_1/amd$, $I4_1/acd$
Trigonal–hexagonal	3	$P3$, $P3_1$, $P3_2$, $R3$
	$\bar{3}$	$P\bar{3}$, $R\bar{3}$
	32	$P312$, $P321$, $P3_112$, $P3_121$, $P3_212$, $P3_221$, $R32$
	3m	$P3m1$, $P31m$, $P3c1$, $P31c$, $R3m$, $R3c$
	$\bar{3}m$	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$, $R\bar{3}m$, $R\bar{3}c$
	6	$P6$, $P6_1$, $P6_5$, $P6_3$, $P6_2$, $P6_4$
	$\bar{6}$	$P\bar{6}$
	$6/m$	$P6/m$, $P6_3/m$
	622	$P622$, $P6_122$, $P6_522$, $P6_222$, $P6_422$, $P6_322$
	6mm	*P6mm*, *P6cc*, $P6_3cm$, $P6_3mc$
	$\bar{6}\,m$	$P\bar{6}2m$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$,
	6/mmm	$P6/mmm$, $P6/mcc$, $P6_3/mcm$, $P6_3/mmc$
Cubic	23	$P23$, $F23$, $I23$, $P2_13$, $I2_13$
	$m\,\bar{3}$	$Pm\bar{3}$, $Pn\bar{3}$, $Fm\bar{3}$, $Fd\bar{3}$, $Im\bar{3}$, $Pa\bar{3}$, $Ia\bar{3}$
	432	$P432$, $P4_232$, $F432$, $F4_132$, $I432$, $P4_332$, $P4_132$, $I4_132$
	$\bar{4}3m$	$P\bar{4}3m$, $F\bar{4}3m$, $I\bar{4}3m$, $P\bar{4}3n$, $F\bar{4}3c$, $I\bar{4}3d$
	$m\bar{3}m$	$Pm\bar{3}m$, $Pn\bar{3}n$, $Pm\bar{3}n$, $Pn\bar{3}m$, $Fm\bar{3}m$, $Fm\bar{3}c$, $Fd\bar{3}m$, $Fd\bar{3}c$, $Im\bar{3}m$, $Ia\bar{3}d$

(2) Projection of the symmetry elements of the space group along special axes (high symmetry). The origin is in the upper left corner.
(3) Projection of a general position.
(4) Information for the selection of the origin.
(5) Asymmetric unit.
(6) Symmetry operations of the space group.
(7) General and special positions, multiplicity Wyckoff letter, site symmetry, and coordinates of equivalent positions.

Patterson symmetry is the symmetry of the Patterson function for Fourier transformation and Wyckoff letter provides the equivalent positions in a unit cell. More details are obtained from the International Tables for Crystallography.

The first alphabetical capital letter is to show the lattice symbol of the Bravais lattices (***P, F, I, A, B, C,*** and ***R***) as summarized in Table 6.3 and next three characters indicate symmetry elements related to the particular orientation in crystal systems as summarized in Table 6.4. For example, we find ***Cmm2*** (orthorhombic) in the International Tables, Vol.A, p.238. This ***Cmm2*** shows that space lattice is base-centered (***C***) and next three characters of ***mm2*** inform us the symmetry elements with respect to directions of [100], [010], and [001], respectively. That is, this orthorhombic space lattice shows mirror plane *m*, perpendicular to both ***a***- and ***b***-axes and a twofold rotation axis along the ***c***-axis. For another example, $\boldsymbol{P12_1/c1}$ (monoclinic) found in the International Tables, Vol.A, p.184 shows that space lattice is primitive (simple) and it has the $\mathbf{2_1}$ screw axis parallel to ***b***-axis and the ***c***-glide plane which is perpendicular to the $\mathbf{2_1}$ screw axis. Since the description of space groups is generally used in a simplified form as much as possible, so-called short space group symbol, for example, $\boldsymbol{P12_1/c1} \rightarrow \boldsymbol{P2_1/c}$ and $\boldsymbol{F}\,4/\boldsymbol{m}\bar{3}\,2/\boldsymbol{m} \rightarrow \boldsymbol{Fm}\bar{3}\,\boldsymbol{m}$ (see Vol. A, p. 688). Then, the users are requested to get familiar with the relationships between symbols and crystal systems including image of atomic positions. Practice makes perfect (see Questions 6.1–6.6).

Table 6.3 Number and coordinates of the lattice points in the unit cells of Bravais lattices

Lattice symbols	No. of lattice points in a unit cell	Coordinates of lattice points in a unit cell
P	1	0,0,0
A	2	$0,0,0\ ;\ 0,\frac{1}{2},\frac{1}{2}$
B	2	$0,0,0\ ;\ \frac{1}{2},0,\frac{1}{2}$
C	2	$0,0,0\ ;\ \frac{1}{2},\frac{1}{2},0$
I	2	$0,0,0\ ;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}$
R	3	$0,0,0\ ;\ \frac{2}{3},\frac{1}{3},\frac{1}{3}\ ;\ \frac{1}{3},\frac{2}{3},\frac{2}{3}$
F	4	$0,0,0\ ;\ \frac{1}{2},\frac{1}{2},0\ ;\ \frac{1}{2},0,\frac{1}{2}\ ;\ 0,\frac{1}{2},\frac{1}{2}$

Table 6.4 The order of Hermann–Mauguin symbols and their relation to directions in a crystal

Crystal systems	1st index	2nd index	3rd index
Triclinic	None		
Monoclinic	[010](*b-axis*)*		
	[001](*c-axis*)*		
Orthorhombic	[100]	[010]	[001]
Tetrogonal	[001]	$\{[100]\ [010]\}$	$\{[1\bar{1}0]\ [110]\}$
Trigonal Referred to hexagonal axes	[001]	$\{[100]\ [010]\ [\bar{1}\bar{1}0]\}$	
Trigonal Referred to rhombohedral axes	[111]	$\{[1\bar{1}0]\ [01\bar{1}]\ [\bar{1}01]\}$	
Hexagonal	[001]	$\{[100]\ [010]\ [\bar{1}\bar{1}0]\}$	$\{[1\bar{1}0]\ [120]\ [\bar{2}\bar{1}0]\}$
Cubic	$\{[100]\ [010]\ [001]\}$	$\{[111]\ [1\bar{1}\bar{1}]\ [\bar{1}1\bar{1}]\ [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0]\ [110]\ [01\bar{1}]\ [011]\ [\bar{1}01]\ [101]\}$

* Orthogonal axis = Unique axis.

The International Tables do not cover only Vol.A focusing on symmetry of space groups, but also Vol.B published in 2001 covering information about the reciprocal lattice, structure factor, Fourier transform, and others including structural analysis by diffuse scattering, dynamical theory, and its applications. One can also find Vol.C, Third Edition in 2004 providing mathematical, physical, and chemical tables including absorption coefficients and X-ray atomic scattering factors. This volume includes sample preparation techniques, methods for the determination of lattice parameters, refining techniques for the structure determination. Further, Vol. D published in 2003 Physical Properties of Crystals, Vol.E in 2002, Sub-periodic Groups, Vol. F in 2001 Crystallography of Biological Macromolecules, and Vol.G in 2005, Definition and Exchange of Crystallographic Data. There is also A1, "Symmetry relations between space groups" published in 2004. It should be suitably selected, depending on the purpose.

6.3 Solved Problems (8 Examples)

Question 6.1 Explain screw axes and glide planes which are important for analyzing the three-dimensional regular array in crystal lattice.

Answer 6.1 A three-dimensional periodic array in crystals is known to be reproduced by the infinite repetition of identical structural units, but we find the following problem.

When supposing an operation around a point brings it to self-coincidence, it is difficult to distinguish between the result obtained by the one cycle operation and that where it returns to the original position from another lattice point separated with several cycles. For this purpose, the operations of rotation and translation may be linked with one another. This is particularly true for the space groups of centered lattices. That is, it is necessary to introduce screw rotation and glide reflection.

The screw axis may be denoted by n_m and its operation is to translate by (m/n) times the length of a unit lattice vector along the direction of a rotation axis every one operation about the n-axis of rotation. As a specific example, a comparison is made in Fig. 1 using the relationships between twofold rotation axis and twofold screw rotation axis. In the operation of twofold screw rotation axis (2_1), the point alters from A to B due to a translation operation applied by half of a unit lattice translation along the direction parallel to the long-axis after the 180° rotation as similar to the twofold rotation axis case and if the same operation is repeated, the point A does not return to its starting point. This operation does not come into coincidence with itself. The point A moves the point corresponding to the position applied by a unit lattice translation along the direction parallel to the long axis.

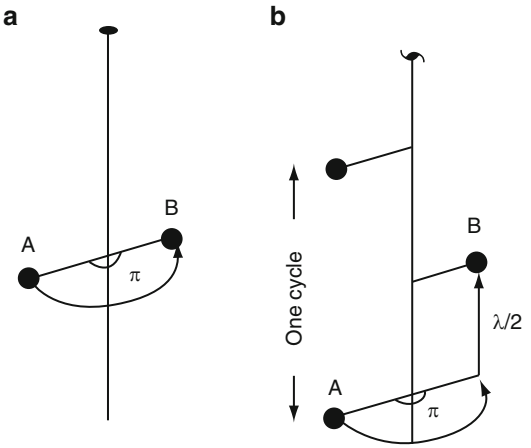


Fig. 1 Twofold rotation axis (**a**) and twofold screw rotation axis (**b**)

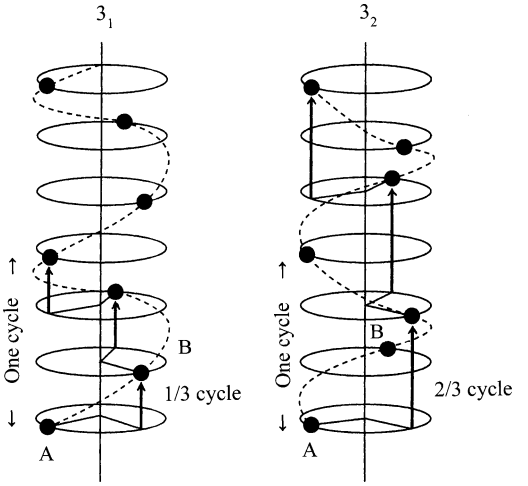


Fig. 2 Threefold screw axes

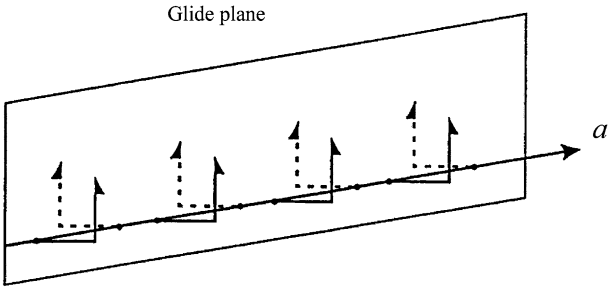


Fig. 3 Example of a glide reflection operation denoted by "a-glide plane"

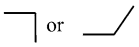
In the operation of threefold screw rotation axis, a translation operation is made by 1/3 of a unit lattice translation along the direction of a rotation axis after every 120° rotation. However, as shown in Fig. 2, keep in mind that there are two ways like the treads of a spiral staircase, clockwise and counterclockwise. In order to distinguish these two cases, the threefold screw rotation axis describes clockwise (3_1) and counterclockwise (3_2). It may be added that there are three fourfold screw rotation axes and five sixfold screw rotation axes (see Fig. 6.3) and screw rotation axes are only allowed in crystals parallel to those directions possibly accepted for rotation axes in the corresponding point group.

Glide plane is divided into three categories; axial glide plane and diagonal and diamond glide plane. Reflection across the so-called mirror plane is followed by translation parallel to the plane by one-half of the length of a unit lattice translation vector. For example, "a-glide plane" is the case where it projects on a mirror surface in pairs and a translation operation by ($\frac{1}{2}\boldsymbol{a}$) is made along the direction parallel to the mirror surface (see Fig. 3). Similarly, there are axial b-glide plane and c-glide plane.

In other words, glide planes are designated by symbols suggesting the relationships of their glide components to the unit lattice vectors.

The n-glide plane is characterized by a translation operation along the diagonal direction. In addition, the diamond glide plane denoted by d-glide plane features one-quarter (1/4) of a lattice translation along the line parallel to the body-centered direction. Symbols and relevant information of these glide planes including a mirror plane are summarized in Table 1.

Table 1 Symbols and their relevance for glide planes including a mirror plane

Symbols	Graphic symbols		Glide plane direction and translation		Limiting conditions
m		⊥ paper	—		—
	 or	∥ paper	—		—
a		⊥ paper	$(h0l)$	$a/2$	$h0l : h = 2n$
		∥ paper	$(hk0)$	$a/2$	$hk0 : h = 2n$
b		⊥ paper	$(0kl)$	$b/2$	$0kl : k = 2n$
		∥ paper	$(hk0)$	$b/2$	$hk0 : k = 2n$
c		⊥ paper ⊥ paper	$(0kl)$ $(h0l)$	$c/2$ $c/2$	$0kl : l = 2n$ $h0l : l = 2n$
n		⊥ paper ⊥ paper	$(0kl)$ $(h0l)$	$(b + c)/2$ $(c + a)/2$	$0kl : k + l = 2n$ $h0l : l + h = 2n$
		∥ paper	$(hk0)$	$(a + b)/2$	$hk0 : h + k = 2n$
d		⊥ paper ⊥ paper	$(0kl)$ $(h0l)$	$(b \pm c)/4$ $(c \pm a)/4$	$0kl : k + l = 4n$ $h0l : l + h = 4n$
		∥ paper	$(hk0)$	$(a \pm b)/4$	$hk0 : h + k = 4n$

Question 6.2 A crystal structure is known to be characterized by points in an infinite three-dimensional regular array. Explain the geometry of crystals using symmetry elements. Keep in mind the viewpoint of symmetry given in a crystal structure, not the mathematical issue.

Answer 6.2 In crystals, a three-dimensional periodic arrangement of atoms is always present and such nature is represented by points. The concept of a lattice corresponding to a three-dimensional periodic arrangement of points is a purely mathematical subject, but it is well accepted as the space lattice. In this case, we use lattice translation for the repetition operation. However, we find other repetition methods called symmetry operations. For example, it is relatively easy to understand the rotation operation as illustrated in Figs. 1 and 2. An operation is required to bring a point into coincidence with itself, such as rotation about an axis and reflection in a plane. When a symmetry operation gives a locus, such as a point, a line, or a plane which is left unchanged by this operation, the locus is referred to as the symmetry element. Note that symmetry may be defined as that spatial property of a pattern or body by which the pattern or body can be brought from a starting state to another indistinguishable state by a certain operation. A symmetry element is also considered to a geometrical entity (point, line, or plane) in a pattern or body, A point is a dimensionless entity in space with coordinates that specify its position. An axis is a line joining two points and a plane is formed by two intersecting lines.

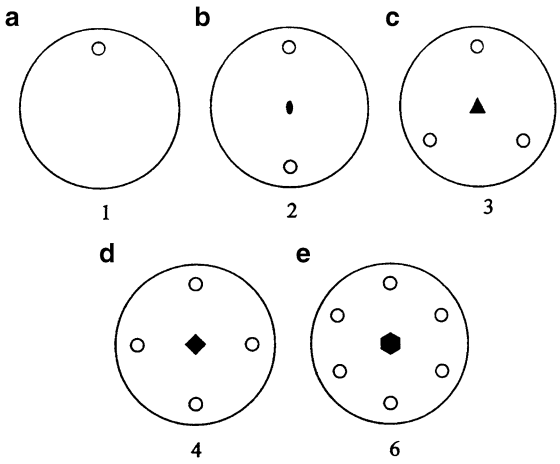


Fig. 1 Point groups having only rotation as symmetry element

Seven crystal systems, each related to the type of unit cell, are combined with 32 point groups which are associated with elements of symmetry in the unit cell itself. Note that the symmetry elements enable us to represent all the possible point arrangements, although a real crystal is a single, unrepeated object. Anyway, with respect to the components of symmetry element, we may suggest a center of symmetry, $\bar{1}$, (or a roto-inversion center), a mirror plane, glide planes, rotation axes, screw axes, and inversion axes. For example, the point which does not move in the inversion operation is called "inversion center." The operation-related mirror plane is given as follows. Any point on one side of a mirror plane is matched with an equivalent point on the other side at the same distance from the plane along a line

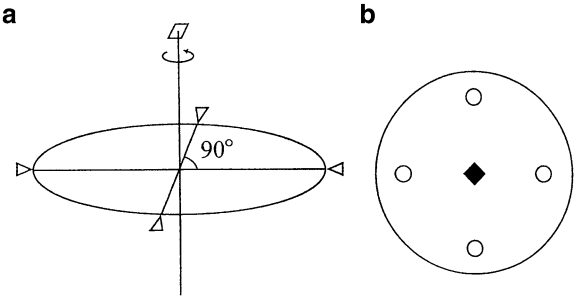


Fig. 2 Fourfold rotation axis (**a**) and its notation (**b**)

normal to it. In other words, the mirror reflection is to match any point or any object with the case where it is reversed after rotating 180° about a twofold axis perpendicular to the target plane. Similarly, the inversion operation can be combined with other axes of rotation called "rotatory-inversion" and this case is also called "onefold rotatory-inversion."

Considering all these factors, we may conclude for symmetry in the following. For the symmetry elements allowed in a three-dimensional periodic arrangement of points, we find ten different ways of "rotation and rotatory inversion" without translation; namely, the rotation axes of one, two, three, four, and sixfold rotation axes, as expressed by n and the rotatory inversion (roto-inversion) axes of $\bar{2}, \bar{3}, \bar{4}, \bar{6}$ denoted by $\bar{n}$. However, it is rather stressed here that there are only EIGHT independent symmetry elements by excluding threefold rotatory-inversion axis ($\bar{3}$) and sixfold rotatory-inversion axis ($\bar{6}$).

In other words, it is found out that there are 32 point groups for covering a three-dimensional periodic arrangement of points in space lattice using these eight symmetry elements and their combinations. Some key points for point groups are summarized as follows.

(1) Point groups where only rotation is recognized as a symmetry element (five cases: 1, 2, 3, 4, and 6).
(2) Point groups where only axis of rotatory-inversion is recognized as symmetry element (five cases: $\bar{1}$, $\bar{2} = m$, $\bar{3}$, $\bar{4}$, and $\bar{6} = 3/m$).
(3) Point groups where n-fold rotation axis is perpendicular to twofold rotation axis (four cases: 222, 32, 422, and 622).
(4) Point groups which have a mirror plane perpendicular to the n-fold rotation axis (three cases: $2/m$, $4/m$, and $6/m$).
(5) Point groups which have a mirror plane parallel to the n-fold rotation axis (four cases: $2mm$, $3m$, $4mm$, and $6mm$).
(6) Point groups of 222, 32, 422 and 622 (corresponding to the No.3 cases), when further considering a mirror plane perpendicular to the n-fold rotation axis (four cases: mmm, $\bar{6}m2$, $4/mmm$ and $6/mmm$).
(7) Point groups of 222 and 32 (corresponding to the No.3 case), when further considering a mirror planes so as to bisect an angle formed by twofold rotation axes parallel to the plane of drawing (two cases: $\bar{4}2m$ and $\bar{3}m$).

(8) Point group where four threefold rotation axes mutually intersect to make the tetrahedral angle of 109.471° (one case only: 23). Similarly, point group where four threefold rotation axes mutually intersect to make the octahedral angle of 70.529° (one case only: 432).
(9) Point groups of 23 and 432 (corresponding to the No.8 case), when further considering several mirror planes (three cases: $m3$, $\bar{4}3m$, and $m3m$).

In order to represent the 32 point groups, we find two methods, Schöenflies and Hermann–Mauguin symbols. Although Schönflies symbols are widely used in the field of spectroscopy, especially of organic molecules, the use of Hermann–Mauguin symbols become popular in crystallography, because of the IUCr suggestion. If need, we can use the results summarized in Table 1. It may also be noteworthy that the abbreviation form is generally used in cases possibly described by combination of higher symmetry. For example, in the point group of $4\bar{3}2$ for a cube described by a combination of symmetry operations of fourfold, threefold, and twofold axes, the best description for symmetry is given by two mirror planes; one is $4/m$ perpendicular to fourfold axis and another is $2/m$ perpendicular both to threefold rotatory-inversion axis $\bar{3}$ and twofold axis. In this case, the original full-notation is $\frac{4}{m}\bar{3}\frac{2}{m}$, but the abbreviation form of m$\bar{3}$m is widely employed. Some helpful information can be obtained from the results of Table 2.

The following information may be convenient in the symmetry operations for crystallography. When including translation, it is necessary to consider "screw axes" with translation to the direction of rotation and its axis and a mirror plane and a "glide plane" with translation parallel to it. Keeping these factors in mind, it is necessary to stipulate the direction of an axis as well as the direction of the translational operation, so that the combination of eleven screw axes and five glide planes as listed in Table 3 may be linked with one another.

Table 1 Hermann–Mauguin and Schöenflies symbols for the 32 crystallographic point groups

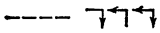
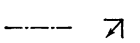
Harmann–Mauguin symbols	Schöenflies symbols	Harmann–Mauguin symbols	Schöenflies symbols	Harmann–Mauguin symbols	Schöenflies symbols
1	C_1	4 2 2	D_4	$6/m$	C_{6h}
$\bar{1}$	C_i	$4mm$	C_{4v}	6 2 2	D_6
2	C_2	$\bar{4}$ 2 m	$D_{2\alpha}$	6 m m	C_{6v}
m	C_s	$4/mmm$	D_{4h}	$\bar{6}$ m 2	D_{3h}
$2/m$	C_{2h}	3	C_3	$6/mmm$	D_{6h}
2 2 2	D_2	$\bar{3}$	C_{3i}	2 3	T
mm 2	C_{2v}	3 2	D_3	$\bar{m}$ 3	T_h
mmm	D_{2k}	3 m	C_{3v}	432	O
4	C_4	$\bar{3}$ m	$D_{3\alpha}$	4 3 m	T_α
$\bar{4}$	S_4	6	C_6	m 3 m	O_h
$4/m$	C_{4h}	$\bar{6}$	D_{3h}		

Table 2 The 32 point groups and their relation to the crystal systems

Crystal system	Point groups	
Triclinic	$\bar{1}$	1
Monoclinic	$2/m$	m,2
Orthorhombic	$2/m\ 2/m\ 2/m$ (mmm)	$mm2$, 222
Tetragonal	$4/m\ 2/m\ 2/m$ ($4/mmm$)	$\bar{4}2m$, $4mm$, 422 $4/m$, $\bar{4}$, 4
Trigonal	$\bar{3}2/m$ ($\bar{3}m$)	$3m$, 32, $\bar{3}$, 3
Hexagonal	$6/m\ 2/m\ 2/m$ ($6/mmm$)	$\bar{6}m2$, $6mm$, 622 $6/m$, $\bar{6}$, 6
Cubic	$4/m$, $\bar{3}\ 2/m$ ($m\bar{3}m$)	$\bar{4}3m$, 432, $2/m\ \bar{3}$, 23 ($m\bar{3}$)

( ): abbreviated symbols.

Table 3 Symbols and their relevance of symmetry elements including translation

Symbol	Symmetry elements	Graphical symbol	Translation
2_1	2-fold screw		$c/2$, $a/2$ or $b/2$
3_1	3-fold screw		$c/3$
3_2			$2c/3$
4_1	4-fold screw		$c/4$
4_2			$2c/4$
4_3			$3c/4$
6_1	6-fold screw		$c/6$
6_2			$2c/6$
6_3			$3c/6$
6_4			$4c/6$
6_5			$5c/6$
a, b	Glide plane		Translation parallel to the plane of paper ($a/2$, $b/2$ etc.)
c			Translation perpendicular to the plane of paper ($c/2$ etc.)
n	Diagonal glide plane		$(a+b)/2$ etc.
d	Diamond glide plane		$(a+b)/4$ etc.

Question 6.3 The mathematical concept of space groups is used for structural analysis of crystals. Explain the space groups using a monoclinic system as an example.

Answer 6.3 Usually more than one symmetry element is present in crystals. For crystals, only the rotational values $n = 1, 2, 3, 4$, and 6 are permitted and 32 crystallographic point groups are generated. Point groups are the symmetry groups of a finite body, but space groups should be described as an infinite set of symmetry elements. That is, space groups provide the symmetry not only of crystal lattices but also of crystal structures.

When 32 point groups are analyzed and arranged on the basis of degrees of rotation axis, all crystals are known to be classified into one of the seven crystal systems. Furthermore, the periodic sequence found in crystals has been systematically analyzed using all symmetry operations possible; four symmetry operations of mirror reflection, rotation, inversion and rotatory-inversion and eleven screw axes and five translational operations of glide planes and their combinations and then we obtain the 230 space groups. Combinations of these 230 space groups are proved from purely mathematical point of view. In other words, any periodic arrangement found in crystals can be expressed by one of the 230 space groups.

In the monoclinic system, the lattices are characterized by two unit cell descriptions; simple lattice (P) which has only one lattice point in a unit cell and one centered lattice (C) which has a lattice point at the center of the ab-plane. Point groups are 2, m, and $2/m$. For example, let us consider the case of P and C with a point group of 2, we obtain four combinations such as $P2$, $C2$, $P2_1$, and $C2_1$. However, $C2$ is equivalent to $C2_1$, as readily seen from the results of Fig. 1, so that this combination provides three space groups denoted by $P2$, $C2$, and $P2_1$.

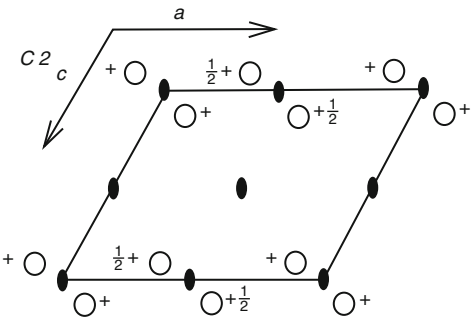


Fig. 1 The operation of the space group $C2$

Since one screw axis and one glide-plane (c-glide plane in this case) will be taken into consideration, we have to check the following five cases of 2_1, c, $2_1/m$, $2/c$, and $2_1/c$. Taking all these factors, the 13 combinations are found to be possible as the space lattices P and C of the monoclinic system. The results are summarized in Table 1 together with subgroups of $P2/m$ and $C2/m$. Note that we also find the relationships of $C2_1 = C2/m$, $C2_1/c = C2/c$, and $C2_1 = C2$.

All possible space groups of the monoclinic system can be derived in a slightly different way. Starting from the two monoclinic space groups of highest symmetry of $P2/m$ and $C2/m$. In $C2/m$, there are a-glide planes at $(x, 1/4, z)$ and $(x, 3/4, z)$ and 2_1-axes at $(1/4, y, 0)$, $(1/4, y, 1/2)$, $(3/4, y, 0)$, and $(3/4, y, 1/2)$.

The monoclinic subgroups for the point group $2/m$ are m and 2. Then, the replacement of point symmetry elements of 2 and m can be done by using 2_1 and a-glide plane, respectively. Since m is parallel to the plane denoted by (010), only a-, c-, and n-glide planes are possible. However, a different selection of the a- and c-axes will convert either a-glide or n-glide into c-glide plane. For this reason we need to take only the c-glide plane into account. Accordingly, the replacement of 2 and m by 2_1 and c results in the 13 monoclinic space groups as summarized in Table 1.

Table 1 Space and point groups for the monoclinic crystal system

Point groups	Space groups	
$2/m$	$P2/m$	$C2/m$
	$P2_1/m$	$C2_1/m^* \equiv C2/m$
	$P2/c$	$C2/c$
	$P2_1/c$	$C2_1/c^* \equiv C2/c$
m	Pm	Cm
	Pc	Cc
2	$P2$	$C2$
	$P2_1$	$C21^* \equiv C2$

When the point symmetry elements 2 and m is replaced by 2_1, a screw axis always appears between the twofold rotation axes, so that the symmetry element of 2_1 has been excluded in the centered-lattice (C) case. In other words, a- and n-glide planes occur in the C-centered space group case, so that the pairs of symbols $C2_1/m = C2/m$, $C2_1/c = C2/c$, and $C2_1 = C2$ give only a single space group each. Similarly, the same combination may be considered about other crystal systems and it is quite complicated as actual work. Since this point is purely handled as mathematical issue and the answer (restricted to 230 cases) has already come out, we should use the result. Detailed information of these 230 space groups are available in the International Tables, Volume A with the chart showing an equivalent positions in a unit cell.

For convenience, Table 2 shows the space group symbols for the 14 Bravais lattices.

Table 2 The space group symbols for the 14 Bravais lattices

	P	C	I	F
Triclinic	$P\bar{1}$			
Monoclinic	$P2/m$	$C2/m$		
Orthorhombic	$P2/m\ 2/m\ 2/m$	$C2/m\ 2/m\ 2/m$	$I2/m\ 2/m\ 2/m$	$F2/m\ 2/m\ 2/m$
Tetragonal	$P4/m\ 2/m\ 2/m$		$I4/m\ 2/m\ 2/m$	
Trigonal	$P6/m\ 2/m\ 2/m$	$R\bar{3}2/m$		
Hexagonal				
Cubic	$P4/m\bar{3}2/m$		$I4/m\bar{3}2/m$	$F4/m\bar{3}2/m$

Question 6.4 Explain the Laue groups which are important as an indicator, when determining the space group of the structure of a desired substance.

Answer 6.4 The periodicity in regular three-dimensional lattice can be analyzed by the concept of symmetry, but one of our main interests in X-ray crystallography is to reveal the structure of the desired substances. This suggests "how to obtain information that the atomic distribution in a crystal of interest is described by one of the 230 space groups and by one of the 32 point groups with sufficient reliability."

Since the measured X-ray diffraction data enable us to provide information of the reciprocal lattices, the symmetry of reciprocal lattices is examined first and then the symmetry of crystals are extracted. The use of centrosymmetric point groups called "Laue groups" is known to be quite useful for this purpose. Figure 1 shows the experimental set-up for taking a Laue photograph on a flat-plate film using a white X-ray source. The crystal is stationary with respect to the X-ray beam, so that the crystal acts as a kind of filter for selecting the correct wavelength for each reflection under the Bragg law. The resultant spots lie on ellipses and all of which have one end of their major axis at the center of the photographic film. All spots on one ellipse arise through reflections from planes that lie in one and the same zone. A diffraction pattern formed by spots is centrosymmetric.

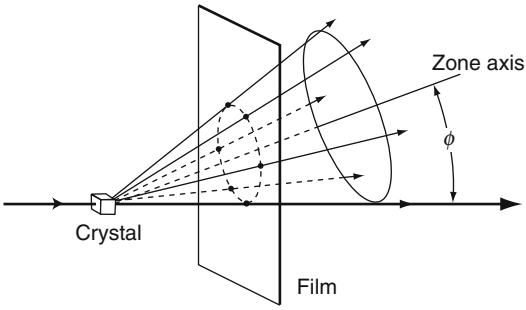


Fig. 1 Schematic diagram for the experimental condition for taking a Laue photograph on a flat-plane film (Transmission type)

Laue photographs using a white X-ray source providing information about symmetry of the weighted reciprocal lattice will reveal the presence of all the symmetry elements associated with the various point groups, but will add a center of symmetry (for noncentrosymmetric point groups). Namely, the arrangement of spots obtained on the Laue photograph exhibits only the symmetry that would be found from a crystal having the corresponding centrosymmetric point groups. There are only eleven possible symmetries and they are called "Laue groups." It may be added that the Laue group assigned to a crystal of interest gives the symmetry of the complete diffraction pattern from that crystal. Thus, the classification of the 32 point

groups is possible by means of the Laue diffraction symmetry as shown in Table 1, where the symmetry of the Laue photographs on a flat-plate film can be described for directions of the incident X-ray beam normal to the crystallographic forms as listed. Note that point group projection symmetry corresponds to the symmetry of the projection of the general form of a point group on to a plane.

Table 1 Crystal systems, Laue groups, and Laue projection symmetry

Crystal systems	Point groups	Laue groups	Laue-projection symmetry normal to the given form		
			$\{100\}$	$\{010\}$	$\{010\}$
Triclinic	1, $\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$
Monoclinic	2, m, 2/m	2/m	m	2	m
Orthorhombic	222, $mm2$, mmm	mmm	$2mm$	$2mm$	$2mm$
			$\{001\}$	$\{100\}$	$\{110\}$
Tetragonal	4, $\bar{4}$, 4/m	4/m	4	m	m
	422, $4mm$ $\bar{4}\,2m$, 4/mmm	4/mmm	$4mm$	$2mm$	$2mm$
			$\{0001\}$	$\{10\bar{1}0\}$	$\{11\bar{2}0\}$
Trigonal*	3, $\bar{3}$	$\bar{3}$	3	1	1
	32, $3m$, $\bar{3}m$	$\bar{3}m$	$3m$	m	2
Hexagonal	6, $\bar{6}$, 6/m	6/m	6	m	m
	622, $6mm$, $\bar{6}\,m2$, 6/mmm	6/mmm	$6mm$	$2mm$	$2mm$
			$\{100\}$	$\{111\}$	$\{110\}$
Cubic	23, $m3$	$m3$	$2mm$	3	m
	432, $\bar{4}3m$, $m3m$	$m3m$	$4mm$	$3m$	$2mm$

[a] Referred to hexagonal axis.

A rotation axis of crystal lattice becomes that of the corresponding reciprocal lattice and the distribution of the weighted reciprocal lattice points usually has a symmetry center. Therefore, a point group appeared in the reciprocal lattice points can be attributed to one of the Laue groups. In this respect, symmetry elements and equivalent positions of the Laue groups are very important fundamental information for structural analysis of crystals by X-ray diffraction. Such information is summarized in Fig. 2a using the method of projection.

These results are obtained in the following procedure. Let us consider the spherical surface passing through a symmetry center and mark the position where a symmetry element and this spherical surface intersect. Then, as shown in Fig. 2b, project the marked positions from right above on the equatorial plane of the sphere.

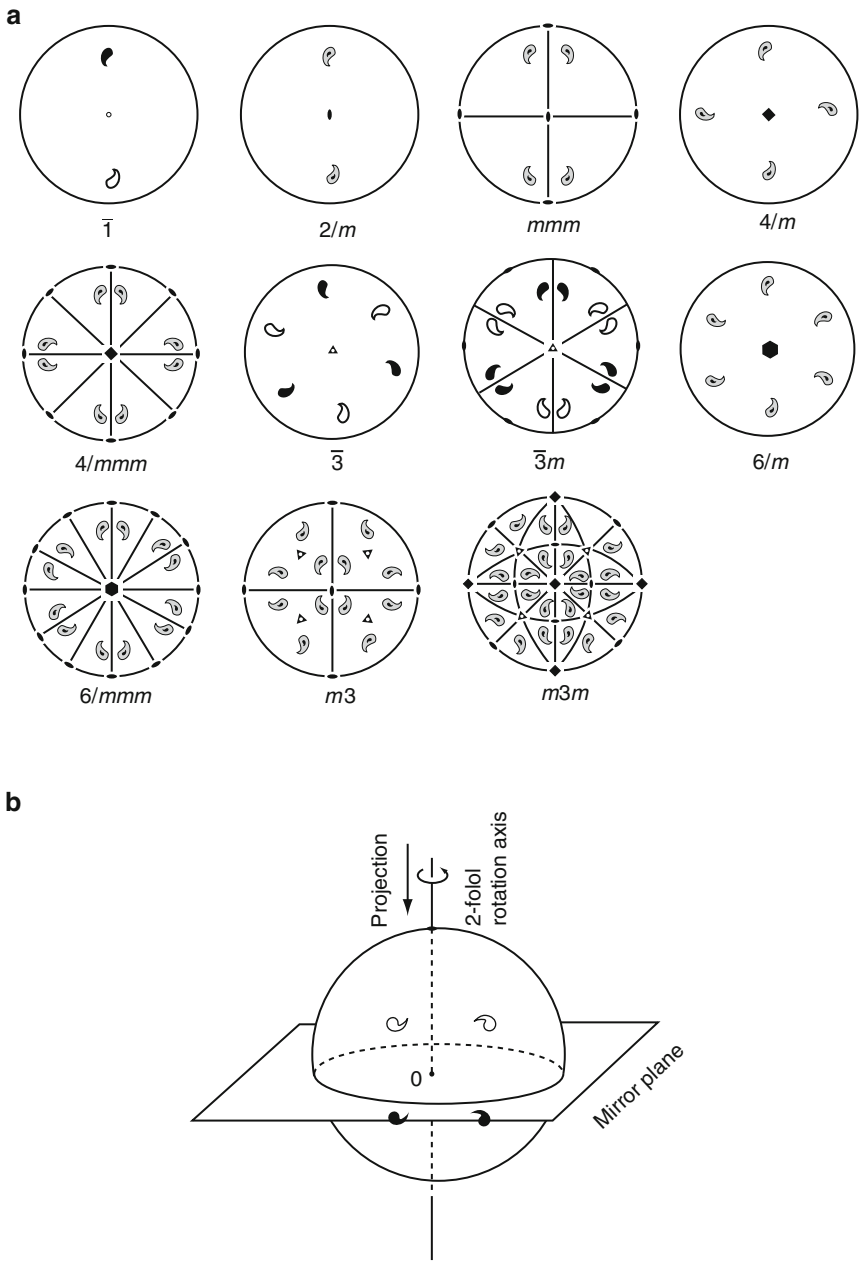


Fig. 2 Symmetry elements and equivalent positions of the Laue group (**a**). Example of projection using the 2/m case (**b**)

The equivalent positions are displayed by a huge comma, and its top surface is colored in white and its bottom in black. If the mirror plane is situated on the equatorial plane, two marks overlap each other upside down on the plane as they are projected. Such overlap is illustrated by black and white overlaid in the figure. Note that the circumference of a circle drawn by thick line indicates that a mirror plane is on the paper surface, the lines other than the circumference show the crossing section between the mirror plane and the sphere by projection.

Question 6.5 Show the variation of Hermann–Mauguin symbol, when the axes of the space group of ***Pnma*** (orthorhombic) are altered within a unit cell. In the same way, show the results of the space group given by $\boldsymbol{Pna}2_1$ (orthorhombic).

Answer 6.5 Let us consider the variation expressed by $\boldsymbol{abc} \rightarrow \boldsymbol{b\bar{a}c} \rightarrow \boldsymbol{\bar{c}\bar{a}b} \rightarrow \boldsymbol{\bar{c}ba} \rightarrow \boldsymbol{bca} \rightarrow \boldsymbol{a\bar{c}b}$, when the starting axis is set to ***abc***. In this case, keep in mind that the origin, O, should be positioned at the top-left corner and further set ***b***-axis to abscissa (horizontal direction), ***a***-axis to ordinate (vertical direction), and ***c***-axis to perpendicular direction to the plane of the drawing in the right-handed system. As shown in Fig. 1, this corresponds to the case of watching a crystal from the right-hand side. While keeping this condition and if every rotat-

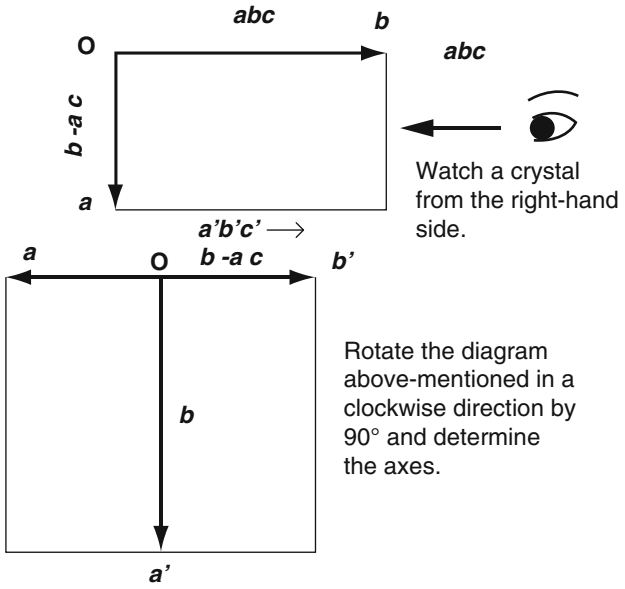


Fig. 1 Fundamentals for changing axes with respect to the orthorhombic system

ing the drawing clockwise by a quarter turn (90°) as shown in Fig. 1, decide axes of $\boldsymbol{a}'$, $\boldsymbol{b}'$, $\boldsymbol{c}'$. Such processes are summarized in Fig. 2. For convenience, Fig. 3 also shows the results using the conversion relationships between ***Pnma*** and ***Pbnm*** when changing the axes from ***abc*** in ***Pnma*** to $\overline{\boldsymbol{c}}\boldsymbol{ab}$ in ***Pbnm***, as an example.

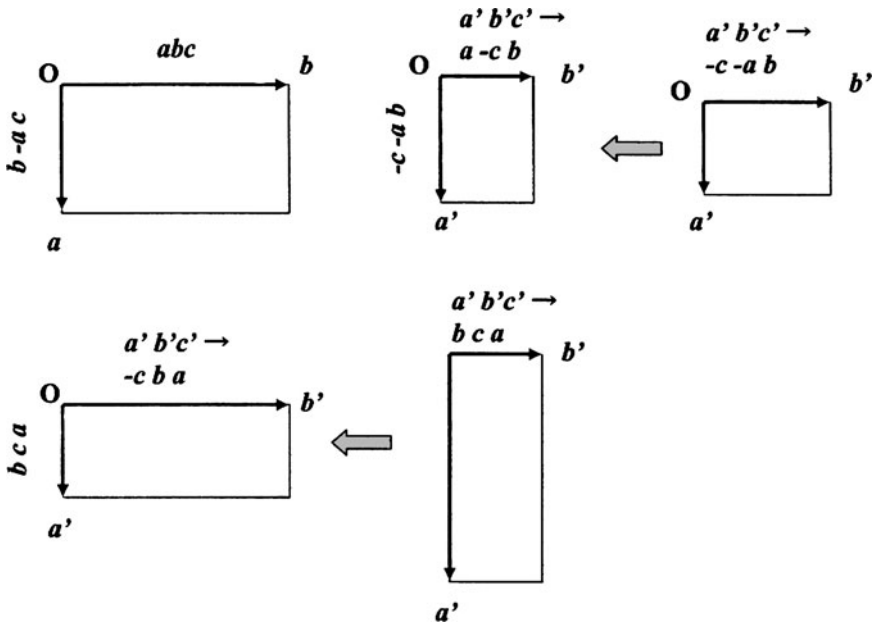


Fig. 2 Variations due to $abc \rightarrow b\bar{a}c \rightarrow \bar{c}ab \rightarrow \bar{c}ba \rightarrow bca \rightarrow a\bar{c}b$

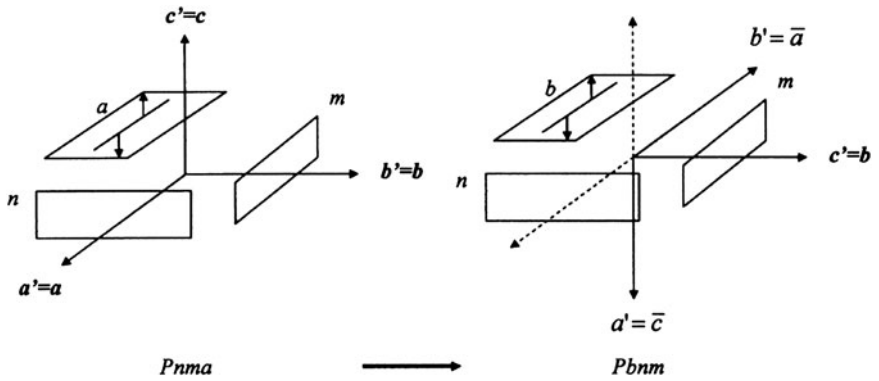


Fig. 3 The relationships between *Pnma* and *Pbnm* due to the change in axes of $abc \rightarrow \overline{c}ab$

The results are summarized as follows.

$$\boldsymbol{abc} \rightarrow \boldsymbol{b\bar{a}c} \rightarrow \boldsymbol{\bar{c}\bar{a}b} \rightarrow \boldsymbol{\bar{c}ba} \rightarrow \boldsymbol{bca} \rightarrow \boldsymbol{a\bar{c}b}$$

$$\boldsymbol{Pnma}, \boldsymbol{Pbnm}, \boldsymbol{Pmcn}, \boldsymbol{Pnam}, \boldsymbol{Pmnb}, \boldsymbol{Pcmn}$$

$$\boldsymbol{Pna2_1}, \boldsymbol{P2_1nb}, \boldsymbol{Pc2_1n}, \boldsymbol{Pn2_1a}, \boldsymbol{Pbn2_1}, \boldsymbol{P2_1cn}$$

When the crystal axes are altered, we find changes for not only atomic coordinates (x, y, z) but also the basis vectors of reciprocal space $(\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*)$ as well as the reflection indices (hkl) and lattice points (u, v, w). Since information about the axial transformation in each crystal system is provided using matrices in the International Tables, Volume A (see pp.77–89), some additional details are given below.

The general transformation of the coordinate system consists of two parts; a linear part and a shift of origin. The linear part suggests a variation of orientation or length or both of the basis vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$. Note that the shift vector is zero for a purely linear transformation. The 3 rows × 3 columns matrices $\boldsymbol{P}$ of the transformation from $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ to $\boldsymbol{a}', \boldsymbol{b}', \boldsymbol{c}'$ is given using row matrices $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ as follows.

$$(\boldsymbol{a}', \boldsymbol{b}', \boldsymbol{c}') = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})\boldsymbol{P} \tag{1}$$

$$= (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \tag{2}$$

Miller indices of a plane $(h\,k\,l)$ are also given in the same way.

$$(h', k', l') = (h, k, l)\,\boldsymbol{P} \tag{3}$$

Note that the Miller indices are usually made relative prime before and after the transformation.

If using the inverse matrices of $\boldsymbol{P}$ to $\boldsymbol{Q}(= \boldsymbol{P}^{-1})$, the transformation of reciprocal lattice axes, atomic coordinates, and lattice points will be given by the following equation using row matrices, $(\boldsymbol{a}^*/\boldsymbol{b}^*/\boldsymbol{c}^*)$, $(x/y/z)$, and $(u/v/w)$.

$$\begin{pmatrix} \boldsymbol{a}^{*\prime} \\ \boldsymbol{b}^{*\prime} \\ \boldsymbol{c}^{*\prime} \end{pmatrix} = \boldsymbol{Q} \begin{pmatrix} \boldsymbol{a}^* \\ \boldsymbol{b}^* \\ \boldsymbol{c}^* \end{pmatrix} \tag{4}$$

$$= \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \begin{pmatrix} \boldsymbol{a}^* \\ \boldsymbol{b}^* \\ \boldsymbol{c}^* \end{pmatrix} \tag{5}$$

$$\left.\begin{aligned} (x'/y'/z') &= \boldsymbol{Q}(x/y/z) \\ (u'/v'/w') &= \boldsymbol{Q}(u/v/w) \end{aligned}\right\} \tag{6}$$

For convenience, a general comment is supplemented with respect to the case where the axes of a space group are changed within a unit cell. A space group symbol is usually described by four symbols such as ***Pnma*** and ***Cmca***, and they provide the relationship of each symmetry element with respect to the direction of a crystal axis. In other words, a space group symbol such as monoclinic and orthorhombic crystal systems is found to depend on the choice of a crystal axis. However, for crystal systems of relatively high symmetry the selection of a crystal axis does only a small variation in the space group symbol, because the selection of an axis is rather limited. In addition, since the triclinic crystal system has no axial symmetry element, the space group symbol is limited to only $\boldsymbol{P1}$ and $\boldsymbol{P\bar{1}}$.

If $\boldsymbol{b}$-axis is fixed in a monoclinic crystal system, the selection of other two axes is limited to a two-dimensional plane. Thus, it is relatively easy to understand that three kinds of notations given by $\boldsymbol{P2_1/c}, \boldsymbol{P2_1/a}$, and $\boldsymbol{P2_1/n}$ are the same space groups. Whereas, it is not optional how to select an axis as for the orthorhombic crystal system characterized by the three axes which are at right angles to one another (mutually perpendicular). Nevertheless, there are 3 ways of selecting $\boldsymbol{a}$-axis and 2 ways for $\boldsymbol{b}$-axis after fixing $\boldsymbol{a}$-axis, which results in six combinations even if the selection is limited to the right-handed system. Note that the space group symbols related to the axis are just three and the first being the notation to represent centered lattices, the second being the order of appearance of the axis symbol or plane one, and the third being the forward direction of a glide plane. This is applicable to the unit cell transformations. For example, when the directions of three axes in space are numbered as 1, 2, and 3 and each direction is named by $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$, respectively, one can obtain six combinations as summarized in Table 1.

Table 1 Transformations of the crystal axes in the orthorhombic system

	1	2	3	3*m*31
(1)	$\boldsymbol{a}$	$\boldsymbol{b}$	$\boldsymbol{c}$	***Cmca***
(2)	$\boldsymbol{a}$	$\boldsymbol{c}$	$\boldsymbol{-b}$	***Bmab***
(3)	$\boldsymbol{b}$	$\boldsymbol{c}$	$\boldsymbol{a}$	***Abma***
(4)	$\boldsymbol{b}$	$\boldsymbol{a}$	$\boldsymbol{-c}$	***Ccmb***
(5)	$\boldsymbol{c}$	$\boldsymbol{a}$	$\boldsymbol{b}$	***Bbcm***
(6)	$\boldsymbol{c}$	$\boldsymbol{-b}$	$\boldsymbol{a}$	***Acam***

Some additional details for this combinations are given. Let us temporarily assume that the case (1) of Table 1 is given by ***Cmca*** which represents the symbol of space lattice, the first symmetry element, the second symmetry element, and third symmetry element. The symbol of ***Cmca*** is, of course, a temporary one, so that it depends on the method "how to give name an axis." For this reason, $\boldsymbol{3m31}$ related to the directions of three fixed axes 1, 2, and 3 is provided in the top right end of Table 1. As setting is made in this way, six variations will be decided in turn and the resultant symbols will be obtained as shown in the right-end column of Table 1.

For example, since the axis of 3 is given as ***a*** for the case (3), its symbol will be ***Abma*** with ***A*** for the space lattice, ***b*** for the first symmetry element which is the direction of the glide plane for ***a***-axis, ***m*** for the second symmetry element as ***b***-axis matches the axis of 1 and then no change, and ***a*** for the third symmetry element which corresponds to the direction of the glide plane for ***c***-axis.

More information can be obtained from the International Tables for Crystallography.

Question 6.6 Obtain the structure factor of F_{hkl} and $|F_{hkl}|^2$ and show the condition where the diffraction intensity can be observed in the following three cases:

(1) The fourfold rotation axis along the a_3-axis in a unit cell.
(2) The 4_1 screw axis along the a_3-axis in a unit cell.
(3) The 4_2 screw axis along the a_3-axis in a unit cell.

Answer 6.6

(1) The atomic positions in a unit cell with the fourfold rotation axis are given by x, y, z; $\bar{y}, x, z$; $\bar{x}, \bar{y}, z$; and $y, \bar{x}, z$. Then, the structure factors F_{hkl} and $|F_{hkl}|^2$ in this case are computed in the following equations.

$$\begin{aligned} F_{hkl} &= f\mathrm{e}^{2\pi \mathrm{i} l z}\left\{\mathrm{e}^{2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{2\pi \mathrm{i}(kx-hy)} + \mathrm{e}^{-2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{-2\pi \mathrm{i}(kx-hy)}\right\} \\ &= 2f\mathrm{e}^{2\pi \mathrm{i} l z}\{\cos 2\pi(hx+ky) + \cos 2\pi(kx-hy)\} \\ &= 4f\mathrm{e}^{2\pi \mathrm{i} l z}\cos\pi\{(h+k)x-(h-k)y\}\cos\pi\{(h-k)x+(h+k)y\} \end{aligned}$$

$$|F_{hkl}|^2 = 16f^2\cos^2\pi\{(h+k)x-(h-k)y\}\cos^2\pi\{(h-k)x+(h+k)y\}$$

Therefore, there is no condition where the diffraction intensity cannot be detected with respect to the atoms in a unit cell with the fourfold rotation axis.

(2) The atomic positions in a unit cell with the 4_1-screw axis are given by x, y, z; $\bar{y}, x, z+\frac{1}{4}$; $\bar{x}, \bar{y}, z+\frac{1}{2}$; and $y, \bar{x}, z+\frac{3}{4}$. The structure factors for this case are computed as follows.

$$\begin{aligned} F_{hkl} = f\mathrm{e}^{2\pi \mathrm{i} l z}\{&\mathrm{e}^{2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{\mathrm{i}\pi l/2}\mathrm{e}^{2\pi \mathrm{i}(kx-hy)} \\ &+ \mathrm{e}^{\mathrm{i}\pi l}\mathrm{e}^{-2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{\mathrm{i}3\pi l/2}\mathrm{e}^{-2\pi \mathrm{i}(kx-hy)}\} \end{aligned}$$

Here, let us consider the case of $l = 4n$,

$$F_{hkl} = f\mathrm{e}^{2\pi \mathrm{i} l z}\left\{\mathrm{e}^{2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{2\pi \mathrm{i}(kx-hy)} + \mathrm{e}^{-2\pi \mathrm{i}(hx+ky)} + \mathrm{e}^{-2\pi \mathrm{i}(kx-hy)}\right\}$$

$$|F_{hkl}|^2 = 16f^2\cos^2\pi\{(h+k)x-(h-k)y\}\cos^2\pi\{(h-k)x+(h+k)y\}$$

There is no condition where the diffraction intensity cannot be detected, along the way similar to the fourfold rotation axis case.

On the other hand, let us consider the case of $l = 4n \pm 1$, one obtains the following results.

$$F_{hkl} = 2f\,\mathrm{e}^{2\pi \mathrm{i} lz}\{\mathrm{i}\sin 2\pi(hx+ky) \mp \sin 2\pi(kx-hy)\}$$
$$|F_{hkl}|^2 = 4f^2\left\{\sin^2 2\pi(hx+ky) + \sin^2 2\pi(kx-hy)\right\}$$

In addition, the following results are obtained for the case of $l = 4n + 2$.

$$F_{hkl} = 4f\,\mathrm{e}^{2\pi \mathrm{i} lz}\sin\pi\{(h+k)x-(h-k)y\}\sin\pi\{(h-k)x+(h+k)y\}$$
$$|F_{hkl}|^2 = 16f^2\sin^2\pi\{(h+k)x-(h-k)y\}\sin^2\pi\{(h-k)x+(h+k)y\}$$

It is noteworthy from these two results that the diffraction intensity for a peak whose Miller indices are given by $(0\ 0\ l)$ can be observed only under the condition $l = 4n$.

(3) The structure factor F_{hkl} is computed from the atomic positions in a unit cell with the 4_2-screw axis; x, y, z; $\bar{y}, x, z+\frac{1}{2}$; $\bar{x}, \bar{y}, z$; $y, \bar{x}, z+\frac{1}{2}$ in the following form.

$$F_{hkl} = 2f\,\mathrm{e}^{2\pi \mathrm{i} lz}\left\{\cos 2\pi(hx+ky) + \mathrm{e}^{\mathrm{i}\pi l}\cos 2\pi(kx-hy)\right\}$$

When considering $l = 2n$,

$$F_{hkl} = 2f\,\mathrm{e}^{2\pi \mathrm{i} lz}\{\cos 2\pi(hx+ky) + \cos 2\pi(kx-hy)\}$$
$$|F_{hkl}|^2 = 4f^2\{\cos 2\pi(hx+ky) + \cos 2\pi(kx-hy)\}^2$$

When considering $l = 2n + 1$,

$$F_{hkl} = 2f\,\mathrm{e}^{2\pi \mathrm{i} lz}\{\cos 2\pi(hx+ky) - \cos 2\pi(kx-hy)\}$$
$$|F_{hkl}|^2 = 4f^2\{\cos 2\pi(hx+ky) - \cos 2\pi(kx-hy)\}^2$$

In conclusion, the diffraction intensity for a peak whose Miller indices are given by $(0\ 0\ l)$ can be observed only under the condition $l = 2n$.

Question 6.7 Let us consider the monoclinic space group denoted by ***P*2₁/*c***, showing the primitive lattice with the 2_1-fold screw axis parallel to ***b*-**axis, the *c*-glide plane being perpendicular to ***b*-**axis with glide of $\frac{c}{2}$. Answer the following questions.

(1) Illustrate the symmetry of this space lattice such as a symmetry center and show both general position and special positions.
(2) Find the extinction condition.

Answer 6.7

(1) Assuming the 2_1-fold screw axis and the glide plane being perpendicular to ***b***-axis as shown in Fig. 1. In addition, the center of point symmetry (a symmetry center) is indicated by a solid circle at $\frac{1}{4}$ or $\frac{3}{4}$ along the c-axis. If the position of $(0, \frac{1}{4}, \frac{1}{4})$ is set to the symmetry center, we obtain the results of Fig. 2. Therefore, the general positions can be given as follows.

$$x, y, z; \bar{x}, \bar{y}, \bar{z}; \bar{x}, \frac{1}{2} + y, \frac{1}{2} - z; x, \frac{1}{2} - y, \frac{1}{2} + z$$

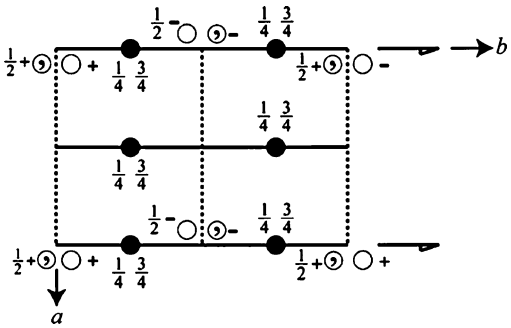


Fig. 1 Monoclinic space lattice. Solid circles indicate symmetry centers

The special positions corresponding to the symmetry center are also given as follows (see solid circles in Fig. 2)

$$(0 \quad 0 \quad 0) : \left(0 \quad \frac{1}{2} \quad \frac{1}{2}\right), \left(\frac{1}{2} \quad 0 \quad 0\right) : \left(\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{2}\right)$$

$$\left(0 \quad 0 \quad \frac{1}{2}\right) : \left(0 \quad \frac{1}{2} \quad 0\right), \left(\frac{1}{2} \quad 0 \quad \frac{1}{2}\right) : \left(\frac{1}{2} \quad \frac{1}{2} \quad 0\right)$$

(2) In order to find the extinction condition, the following formulas for trigonometric functions were used.

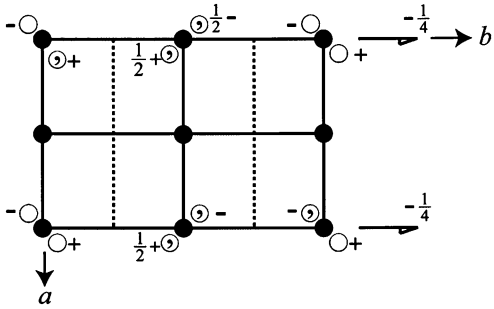


Fig. 2 Monoclinic space lattice when setting a symmetry center to $\left(0, \frac{1}{4}, \frac{1}{4}\right)$. Solid circles indicating a symmetry center at 0 or $\frac{1}{2}$ along the c-axis

$$\begin{cases} \sin A + \sin B = 2\sin\dfrac{A+B}{2}\cos\dfrac{A-B}{2} \\ \cos A + \cos B = 2\cos\dfrac{A+B}{2}\cos\dfrac{A-B}{2} \\ \cos A - \cos B = 2\sin\dfrac{A+B}{2}\sin\dfrac{A-B}{2} \end{cases}$$

The structure factor is computed as follows.

$$\begin{aligned} \frac{F}{f} &= \mathrm{e}^{2\pi\mathrm{i}(hx+ky+lz)} + \mathrm{e}^{2\pi\mathrm{i}(-hx-ky-lz)} \\ &\quad + \mathrm{e}^{2\pi\mathrm{i}\{-hx+k(\frac{1}{2}+y)+l(\frac{1}{2}-z)\}} + \mathrm{e}^{2\pi\mathrm{i}\{hx+(\frac{1}{2}-y)k+(\frac{1}{2}+z)l\}} \\ &= \cos 2\pi(hx+ky+lz) - \mathrm{i}\sin 2\pi(hx+ky+lz) \\ &\quad + \cos 2\pi(-hx-ky-lz) - \mathrm{i}\sin 2\pi(-hx-ky-lz) \\ &\quad + \cos 2\pi\left\{-hx+\left(\frac{1}{2}+y\right)k+\left(\frac{1}{2}-z\right)l\right\} \\ &\quad - \mathrm{i}\sin 2\pi\left\{-hx+\left(\frac{1}{2}+y\right)k+\left(\frac{1}{2}-z\right)l\right\} \\ &\quad + \cos 2\pi\left\{hx+\left(\frac{1}{2}-y\right)k+\left(\frac{1}{2}+z\right)l\right\} \\ &\quad - \mathrm{i}\sin 2\pi\left\{hx+\left(\frac{1}{2}-y\right)k+\left(\frac{1}{2}+z\right)l\right\} \\ &= 2\cos(2\pi,0)\cos 2\pi\frac{2(hx+ky+lz)}{2} \\ &\quad + 2\cos 2\pi\frac{k+l}{2}\cos 2\pi(hx-ky+lz) \end{aligned}$$

$$-\mathrm{i}\sin 2\pi\frac{k+l}{2}\cos(hx-ky+l)$$

$$=2\cos 2\pi(hx+ky+lz)+2\cos 2\pi\frac{k+l}{2}\cos 2\pi(hx-ky+lz)$$

(i) In the case of $k+l=2n$,

$$\frac{F}{f}=4\cos 2\pi(hx+lz)\cos 2\pi ky$$

The extinction does not take place.

(ii) In the case of $k+l=2n+1$,

$$\frac{F}{f}=-4\sin 2\pi(hx+lz)\sin 2\pi ky$$

The extinction takes place under the condition of $h=l=0$ or $k=0$.

Question 6.8 Information about the space group ***Pnma***, No.62 (orthorhombic) can be obtained from the International Tables for Crystallography, Volume A, page 298-299. Explain the key points.

Answer 6.8 The symbol ***Pnma*** described by a shortened form (notation) of Hermann–Mauguin method describes that Bravais lattice is a simple lattice(P) with three symmetry elements ***mnm*** with respect to the direction of [100], [010], and [001] (see Table 6.4). Namely, this orthorhombic has mirror planes perpendicular to these directions. The symbol of D_{2h}^{16} provides the Schöenflies' description and No.62 corresponds to the number allocated in the 230 space groups. Next, ***P*** $2_1/n/2_1/m/2_1/a$ is full expression of three symmetry elements and they are as follows. $2_1/n$ shows the 2_1 screw axis and a diagonal plane of glide reflection perpendicular to it for the direction of ***a***-axis, the $2_1/m$ indicates the 2_1 screw axis and a mirror plane vertical to it for the direction of ***b***-axis, and the $2_1/a$ shows the 2_1 screw axis and a mirror plane perpendicular to it for the direction of ***c***-axis, respectively. The space group of the Patterson function is given by ***Pmmm***. The Patterson function corresponds to the Fourier transform of the square of the structure factor and it is widely used to obtain a map of interatomic distances in the unit cell. In other words, the Patterson function is a superposition of peaks derived from all atomic pairs in the unit cell directly related to the measured diffraction data. (Refer to other textbooks for details of the Patterson function, for example, M.M. Woolfson, An Introduction to X-ray Crystallography, 2nd Edition, Cambridge University Press (1997).)

Four figures are the so-called standard setting of the space group or the space-group tables and first three figures are characterized by the Hermann–Mauguin symbols in the headline. The space-group tables for each orthorhombic space group is known to consist of three projections of the symmetry elements along the ***c***-axis

(upper left), the ***a***-axis (lower left), and the ***b***-axis (upper right), in addition to the general position diagram. For example, with respect to the upper left corner as its origin, the projection is made along the ***c***-axis, setting ***a***-axis and ***b***-axis to the horizontal (abscissa) and the vertical (ordinate) axes, respectively. For convenience, diagrams for the standard setting are shown in Fig. 1 using the orthorhombic and tetragonal space groups as an example, where G = general position diagram. Note that all these figures are described in the right-handed coordinate system.

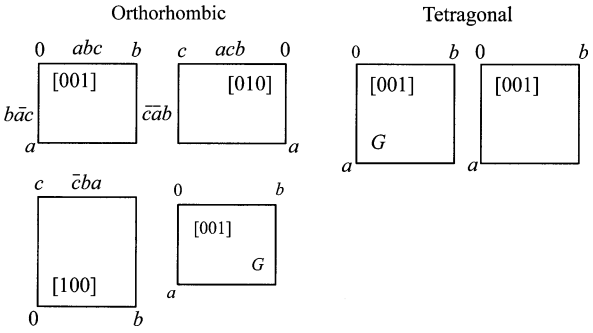


Fig. 1 Diagrams for the standard setting as described in the space-group tables; orthorhombic and tetragonal space groups

For each orthorhombic space group, there are six different ways of assigning the labels ***a, b, c*** to the three orthorhombic symmetry directions. These settings correspond to the six conversions of the labels of the axes including identity conversion. Three space group symbols written on the horizontal axes in three figures of projection are ***Pmnb***, ***Pbnm***, and ***Pmcn*** which are corresponding to the axial conversions of ***abc*** (fundamental axis), ***ac̄b***, and ***c̄ba***. Similarly, ***Pmnb***, ***Pbnm***, and ***Pmcn*** are related to the axial conversions of ***bāc***, ***c̄āb***, and ***bca*** in the vertical axes case. In addition, the numerical value 1/4 placed beside the symmetry element symbols shows the inner height of a unit cell in the projection direction.

The figure at the lower right is corresponding to the general position diagram, which is given only in the projection along ***c***-axis. It may also be suggested that this figure shows the equivalent positions in the same projection as the upper left and provides information about what arrangement of atoms in the general positions will be possible in a unit cell. Both marks ◯ and ⊙ show the equivalent positions and ◯ and ⊙ are related by a mirror plane. They are called enantiomorphs, so that ◯ represents the left-handed system, if ⊙ is given in a right-handed system.

The signs and numerical values, $+, -$ and $\frac{1}{2}+$, $\frac{1}{2}-$ placed beside ◯ are the coordinates to the projection direction of the equivalent positions, and the present case suggests $+z$, $-z$, $\frac{1}{2}+z$, $\frac{1}{2}-z$.

Some other information are summarized as follows.

Origin: The determination of crystal structures is facilitated by the selection of a suitable origin. The line of "Origin" provides the origin selected in the space group

table. According to the International Tables, the position of symmetry center is set to the origin for space groups with a symmetry center and the position of the highest site symmetry becomes the origin for space groups without a symmetry center. In the space group ***Pnma***, the origin is set to a symmetry center denoted by $\bar{\mathbf{1}}$ on the twofold screw axis (as given by "on $\mathbf{1}\ \mathbf{2_1}\ \mathbf{1}$") which is equal to the ***b***-axis.

Asymmetric unit: An asymmetric unit of a space group is considered to be the smallest closed part of space from which by using all symmetry operations, the whole space can be filled. In other words, the line of "Asymmetric unit" shows that the independent area in a unit cell is given in the region; $0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq \frac{1}{4}$, and $0 \leq z \leq 1$ in ***Pnma.***

Symmetry operations: The geometric description of the symmetry operations is given in the space-group tables under the heading "Symmetry operations." These information give a link between the space group diagrams and the general positions. The line of "Symmetry operations" shows the symmetry elements as well as positions related to symmetry operations. In the space group ***Pnma***, symmetry operations of (1)–(8) correspond to eight equivalent positions.

Generators: The line of "Generators" provides all symmetry operations required to generate all equivalent positions of the general positions from coordinates x, y, z. For example, $t(1, 0, 0)$, $t(0, 1, 0)$, and $t(0, 0, 1)$ indicate the translational operation that moves the coordinates x, y, z described by (1) of general positions to the directions of ***a***,- ***b***-, and ***c***-axes by one unit cycle. In the space group ***Pnma***, although symmetry operations of (1)–(8) are cited, all equivalent positions can be generated by operations of (1), (2), (3), and (5). Accordingly, the operations of (4), (6), (7), and (8) are excluded.

Positions: The column of "Position" more explicitly called Wyckoff positions provide information of the equivalent positions when considering site symmetry and are defined as a group of crystalline positions. The following information (a) to (e) classified into general positions and special positions are provided in the space group table.

(a) Multiplicity: This is the number of equivalent points per unit cell and keep in mind it differs from the number of the equivalent lattice planes in one plane of a form called multiplicity factor. The multiplicity of the general position is equal to the order of the point group to which the space group under consideration belongs. On the other hand, the multiplicity of the special position is given by the divisor of multiplicity of the general position. For example, the number of equivalent point in the special position 4*c* is one half of the general equivalent position. This is attributed to the condition that one special position is formed by overlapping two general equivalent positions.
(b) Wyckoff letter: This is simply a coding scheme for the Wyckoff positions. Usually, the notation is made due to the higher degree of site symmetry, starting with *a* at the bottom column for the special position and upward in the alphabetical order traced back to the general position. For example, the general position of

atomic position in the space group ***Pnma*** is $8d$ and its special positions are $4c$, $4b$, $4a$ in order.

(c) Site symmetry: The site symmetry groups of the different points of the same special position are symmetrically equivalent subgroups of the space group and then all points of one special position can be described by the same site symmetry symbol. The column of "Site symmetry" provides the symmetry which the atomic position has. There are two ways in the space group ***Pnma*** where 4 atoms occupy 8 symmetry center sites and the special positions $4a$ and $4b$ correspond to them. There is the mirror symmetry (m) in the special position $4c$. In addition, in order to clarify symmetry directions, the irrelevant axial directions are shown by dots such as *.m*. Here this *.m*. indicates a mirror plane perpendicular to the ***b***-axis.

(d) Coordinates: The sequence of the coordinate triplets is based on the Generators. For centered space groups, the centering translations such as $(0,0,0)+$ $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)+$ are given above the coordinate triplets. The symbol $+$ indicates that the components of the centering translations have to be added to the listed coordinate triplets for obtaining a complete Wyckoff position. Coordinates corresponding to ***a***-, ***b***-, and ***c***-axes with a parallelepiped as a unit cell are referred to as x, y, z. The length of this unit cell is normalized as 1. When one atom exists in the space group ***Pnma***, we find eight atoms without exception at the following positions in a unit cell.
(x,y,z), $\left(-x+\frac{1}{2},-y,z+\frac{1}{2}\right)$, $\left(-x,y+\frac{1}{2},-z\right)$, $\left(x+\frac{1}{2},-y+\frac{1}{2},-z+\frac{1}{2}\right)$, $(-x,-y,-z)$, $\left(x+\frac{1}{2},y,-z+\frac{1}{2}\right)$, $\left(x,-y+\frac{1}{2},z\right)$, $\left(-x+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}\right)$, where $-x$ is $\bar{x}$.

(e) Reflection conditions: Information of the extinction rule is given for the case where atoms are located at the general positions. For example, $0kl : k+l = 2n$ (n is integer) shows, with respect to the $0kl$ reflection, that when $k+l$ is an odd number, its crystal structure factor is zero and if $k+l$ is an even number, it is not zero. On the other hand, when atoms are located only at the special positions, new information of the extinction rule appears in the column listed as Special for every Wyckoff sign, in addition to the conditions given for the general positions. For example, if an atom is only at the $4a$ position, the structure factor becomes zero, when $h+l$ or k is an odd number.
Symmetry of special projections provides information corresponding to two-dimensional space groups and for example, this is used to project the crystal structure with respect to the direction perpendicular to the reciprocal lattices using the two-dimensional intensity data of a zero layer. In each space group table, three different projections are given with respect to the direction indicated by "Along" which is the projection to the plane perpendicular to this direction. Projections depend on crystal system and such information is as follows. Projections are made to the directions of ***c***-, ***a***-, and ***b***-axes for triclinic, monoclinic, and orthorhombic systems. Similarly, the directions of ***c***- and ***a***-axes and [110] for tetragonal system, ***c***- and ***a***-axes and [210] for hexagonal system, [111], [$1\bar{1}0$], and [$2\bar{1}\bar{1}$] for trigonal system and [001], [111], and [110] for cubic system, respectively, are used for the projections. Following the projection

direction, information related to the plane groups generated by the projection of the space groups are provided as the Hermann–Mauguin symbol, $p2gm$, at the present case. In the following line, the relationship with the basic axes $\boldsymbol{a}'$, $\boldsymbol{b}'$ and in the line after that, the origin of plane groups, for example, $(0, 0, z)$ is given using the unit cell coordinates of the space group.