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3.1. Space-group determination and diffraction symbols

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3.1.1. Introduction

In this chapter, the determination of space groups from the Laue symmetry and the reflection conditions, as obtained from diffraction patterns, is discussed. Apart from Section 3.1.6.5, where differences between reflections hkl and $\bar{h}\bar{k}\bar{l}$ due to anomalous dispersion are discussed, it is assumed that Friedel's rule holds, *i.e.* that $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$. This implies that the reciprocal lattice weighted by $|F(hkl)|^2$ has an inversion centre, even if this is not the case for the crystal under consideration. Accordingly, the symmetry of the weighted reciprocal lattice belongs, as was discovered by Friedel (1913), to one of the eleven Laue classes of Table 3.1.2.1. As described in Section 3.1.5, Laue class plus reflection conditions in most cases do not uniquely specify the space group. Methods that help to overcome these ambiguities, especially with respect to the presence or absence of an inversion centre in the crystal, are summarized in Section 3.1.6.

3.1.2. Laue class and cell

Space-group determination starts with the assignment of the *Laue class* to the weighted reciprocal lattice and the determination of the *cell geometry*. The conventional cell (except for the case of a primitive rhombohedral cell) is chosen such that the basis vectors coincide as much as possible with directions of highest symmetry (*cf.* Chapters 2.1 and 9.1).

The axial system should be taken right-handed. For the different crystal systems, the symmetry directions (*blickrichtungen*) are listed in Table 2.2.4.1. The symmetry directions and the convention that, within the above restrictions, the cell should be taken as small as possible determine the axes and their labels uniquely for crystal systems with symmetry higher than orthorhombic. For orthorhombic crystals, three directions are fixed by symmetry, but any of the three may be called a, b or c. For monoclinic crystals, there is one unique direction. It has to be decided whether this direction is called b, c or a. If there are no special reasons (physical properties, relations with other structures) to decide otherwise, the standard choice b is preferred. For triclinic crystals, usually the reduced cell is taken (*cf.* Chapter 9.2), but the labelling of the axes remains a matter of choice, as in the orthorhombic system.

If the lattice type turns out to be centred, which reveals itself by systematic absences in the general reflections hkl (Section 2.2.13), examination should be made to see whether the smallest cell has been selected, within the conventions appropriate to the crystal system. This is necessary since Table 3.1.4.1 for space-group determination is based on such a selection of the cell. Note, however, that for rhombohedral space groups two cells are considered, the triple hexagonal cell and the primitive rhombohedral cell.

The Laue class determines the crystal system. This is listed in Table 3.1.2.1. Note the conditions imposed on the lengths and the directions of the cell axes as well as the fact that there are crystal systems to which two Laue classes belong.

Table 3.1.2.1. *Laue classes and crystal systems*

Laue class	Crystal system	Conditions imposed on cell geometry
$\bar{1}$	Triclinic	None
$2/m$	Monoclinic	$\alpha = \gamma = 90°$ (b unique) $\alpha = \beta = 90°$ (c unique)
mmm	Orthorhombic	$\alpha = \beta = \gamma = 90°$
$4/m$ $4/mmm$	Tetragonal	$a = b; \alpha = \beta = \gamma = 90°$
$\bar{3}$ $\bar{3}m$	Trigonal	$a = b; \alpha = \beta = 90°; \gamma = 120°$ (hexagonal axes) $a = b = c; \alpha = \beta = \gamma$ (rhombohedral axes)
$6/m$ $6/mmm$	Hexagonal	$a = b; \alpha = \beta = 90°; \gamma = 120°$
$m\bar{3}$ $m\bar{3}m$	Cubic	$a = b = c; \alpha = \beta = \gamma = 90°$

3.1.3. Reflection conditions and diffraction symbol

In Section 2.2.13, it has been shown that 'extinctions' (sets of reflections that are systematically absent) point to the presence of a centred cell or the presence of symmetry elements with glide or screw components. Reflection conditions and Laue class together are expressed by the *Diffraction symbol*, introduced by Buerger (1935, 1942, 1969); it consists of the Laue-class symbol, followed by the extinction symbol representing the observed reflection conditions. Donnay & Harker (1940) have used the concept of extinctions under the name of 'morphological aspect' (or aspect for short) in their studies of crystal habit (*cf. Crystal Data*, 1972). Although the concept of aspect applies to diffraction as well as to morphology (Donnay & Kennard, 1964), for the present tables the expression 'extinction symbol' has been chosen because of the morphological connotation of the word aspect.

The *Extinction symbols* are arranged as follows. First, a capital letter is given representing the centring type of the cell (Section 1.2.1). Thereafter, the reflection conditions for the successive symmetry directions are symbolized. Symmetry directions not having reflection conditions are represented by a dash. A symmetry direction with reflection conditions is represented by the symbol for the corresponding glide plane and/or screw axis. The symbols applied are the same as those used in the Hermann–Mauguin space-group symbols (Section 1.3.1). If a symmetry direction has more than one kind of glide plane, for the diffraction symbol the same letter is used as in the corresponding space-group symbol. An exception is made for some centred orthorhombic space groups where *two* glide-plane symbols are given (between parentheses) for one of the symmetry directions, in order to stress the relation between the diffraction symbol and the symbols of the 'possible space groups'. For the various orthorhombic settings, treated in Table 3.1.4.1, the top lines of the two-line space-group symbols in Table 4.3.2.1 are used. In the monoclinic system, dummy numbers '1' are inserted for two directions even though they are not symmetry directions, to bring out the differences between the diffraction symbols for the b, c and a settings.

Example

Laue class: $12/m1$

Reflection conditions:

$hkl: h+k=2n$;
$h0l: h,l=2n$; $0kl: k=2n$; $hk0: h+k=2n$;
$h00: h=2n$; $0k0: k=2n$; $00l: l=2n$.

As there are both c and n glide planes perpendicular to b, the diffraction symbol may be given as $1\,2/m\,1C1c1$ or as $1\,2/m\,1C1n1$. In analogy to the symbols of the possible space groups, $C1c1$ (9) and $C1\,2/c\,1$ (15), the diffraction symbol is called $1\,2/m\,1C1c1$.

For another cell choice, the reflection conditions are:

$hkl: k+l=2n$;
$h0l: h,l=2n$; $0kl: k+l=2n$; $hk0: k=2n$;
$h00: h=2n$; $0k0: k=2n$; $00l: l=2n$.

For this second cell choice, the glide planes perpendicular to b are n and a. The diffraction symbol is given as $1\,2/m\,1A1n1$, in analogy to the symbols $A1n1$ (9) and $A1\,2/n\,1$ (15) adopted for the possible space groups.

3.1.4. Deduction of possible space groups

Reflection conditions, diffraction symbols, and possible space groups are listed in Table 3.1.4.1. For each crystal system, a different table is provided. The monoclinic system contains different entries for the settings with b, c and a unique. For monoclinic and orthorhombic crystals, all possible settings and cell choices are treated. In contradistinction to Table 4.3.2.1, which lists the space-group symbols for different settings and cell choices in a systematic way, the present table is designed with the aim to make space-group determination as easy as possible.

The left-hand side of the table contains the *Reflection conditions*. Conditions of the type $h=2n$ or $h+k=2n$ are abbreviated as h or $h+k$. Conditions like $h=2n, k=2n, h+k=2n$ are quoted as h, k; in this case, the condition $h+k=2n$ is not listed as it follows directly from $h=2n, k=2n$. Conditions with $l=3n$, $l=4n$, $l=6n$ or more complicated expressions are listed explicitly.

From *left* to *right*, the table contains the integral, zonal and serial conditions. From *top* to *bottom*, the entries are ordered such that left columns are kept empty as long as possible. The leftmost column that contains an entry is considered as the 'leading column'. In this column, entries are listed according to increasing complexity. This also holds for the subsequent columns within the restrictions imposed by previous columns on the left. The make-up of the table is such that observed reflection conditions should be matched against the table by considering, within each crystal system, the columns from left to right.

The centre column contains the *Extinction symbol*. To obtain the complete diffraction symbol, the Laue-class symbol has to be added in front of it. Be sure that the correct Laue-class symbol is used if the crystal system contains two Laue classes. Particular care is needed for Laue class $\bar{3}m$ in the trigonal system, because there are two possible orientations of this Laue symmetry with respect to the crystal lattice, $\bar{3}m1$ and $\bar{3}1m$. The correct orientation can be obtained directly from the diffraction record.

The right-hand side of the table gives the *Possible space groups* which obey the reflection conditions. For crystal systems with two Laue classes, a subdivision is made according to the Laue symmetry. The entries in each Laue class are ordered according to their point groups. All space groups that match both the reflection conditions and the Laue symmetry, found in a diffraction experiment, are possible space groups of the crystal.

The space groups are given by their short Hermann–Mauguin symbols, followed by their number between parentheses, except for the monoclinic system, where full symbols are given (*cf.* Section 2.2.4). In the monoclinic and orthorhombic sections of Table 3.1.4.1, which contain entries for the different settings and cell choices, the 'standard' space-group symbols (*cf.* Table 4.3.2.1) are printed in bold face. Only these standard representations are treated in full in the space-group tables.

Example

The diffraction pattern of a compound has Laue class mmm. The crystal system is thus orthorhombic. The diffraction spots are indexed such that the reflection conditions are $0kl: l=2n$; $h0l: h+l=2n$; $h00: h=2n$; $00l: l=2n$. Table 3.1.4.1 shows that the diffraction symbol is $mmmPcn–$. Possible space groups are $Pcn2$ (30) and $Pcnm$ (53). For neither space group does the axial choice correspond to that of the standard setting. For No. 30, the standard symbol is $Pnc2$, for No. 53 it is $Pmna$. The transformation from the basis vectors $\mathbf{a}_e, \mathbf{b}_e, \mathbf{c}_e$, used in the experiment, to the basis vectors $\mathbf{a}_s, \mathbf{b}_s, \mathbf{c}_s$ of the standard setting is given by $\mathbf{a}_s=\mathbf{b}_e, \mathbf{b}_s=-\mathbf{a}_e$ for No. 30 and by $\mathbf{a}_s=\mathbf{c}_e, \mathbf{c}_s=-\mathbf{a}_e$ for No. 53.

Possible pitfalls

Errors in the space-group determination may occur because of several reasons.

(1) *Twinning of the crystal*

Difficulties that may be encountered are shown by the following example. Say that a monoclinic crystal (b unique) with the angle β fortuitously equal to $\sim 90°$ is twinned according to (100). As this causes overlap of the reflections hkl and $\bar{h}kl$, the observed Laue symmetry is mmm rather than $2/m$. The same effect may occur within one crystal system. If, for instance, a crystal with Laue class $4/m$ is twinned according to (100) or (110), the Laue class $4/mmm$ is simulated (twinning by merohedry, *cf.* Catti & Ferraris, 1976, and Koch, 1999). Further examples are given by Buerger (1960). Errors due to twinning can often be detected from the fact that the observed reflection conditions do not match any of the diffraction symbols.

(2) *Incorrect determination of reflection conditions*

Either too many or too few conditions may be found. For serial reflections, the first case may arise if the structure is such that its projection on, say, the b direction shows pseudo-periodicity. If the pseudo-axis is b/p, with p an integer, the reflections $0k0$ with $k \neq p$ are very weak. If the exposure time is not long enough, they may be classified as unobserved which, incorrectly, would lead to the reflection condition $0k0: k=p$. A similar situation may arise for zonal conditions, although in this case there is less danger of errors. Many more reflections are involved and the occurrence of pseudo-periodicity is less likely for two-dimensional than for one-dimensional projections.

For 'structural' or non-space-group absences, see Section 2.2.13.

The second case, too many observed reflections, may be due to multiple diffraction or to radiation impurity. A textbook description of multiple diffraction has been given by Lipson & Cochran (1966). A well known case of radiation impurity in X-ray diffraction is the contamination of a copper target with iron. On a photograph taken with the radiation from such a target, the iron radiation with $\lambda(\mathrm{Fe}) \sim 5/4\lambda(\mathrm{Cu})$ gives a reflection spot $4h_i4k_i4l$ at the position $5h_i5k_i5l$ for copper $[\lambda(\mathrm{Cu}\ K\bar{\alpha})=1.5418\ \mathrm{Å}, \lambda(\mathrm{Fe}\ K\bar{\alpha})=1.9373\ \mathrm{Å}]$. For reflections $0k0$, for instance, this may give rise to reflected intensity at the copper 050 position so that, incorrectly, the condition $0k0: k=2n$ may be excluded.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups*

TRICLINIC. Laue class $\bar{1}$

Reflection conditions	Extinction symbol	Point group	
		1	$\bar{1}$
None	*P*–	*P*1(1)	$P\bar{1}$ (2)

MONOCLINIC, Laue class 2/*m*

Unique axis *b*				Laue class 1 2/*m* 1		
Reflection conditions				Point group		
hkl 0*kl* *hk*0	*h*0*l* *h*00 00*l*	0*k*0	Extinction symbol	2	*m*	2/*m*
			*P*1–1	***P*121** (3)	***P*1*m*1** (6)	***P*1 2/*m* 1** (10)
		k	*P*12$_1$1	***P*12$_1$1** (4)		***P*1 2$_1$/*m* 1** (11)
	h		*P*1*a*1		*P*1*a*1 (7)	*P*1 2/*a* 1 (13)
	h	*k*	*P*1 2$_1$/*a* 1			*P*1 2$_1$/*a* 1 (14)
	l		*P*1*c*1		***P*1*c*1** (7)	***P*1 2/*c* 1** (13)
	l	*k*	*P*1 2$_1$/*c* 1			***P*1 2$_1$/*c* 1** (14)
	h + *l*		*P*1*n*1		*P*1*n*1 (7)	*P*1 2/*n* 1 (13)
	h + *l*	*k*	*P*1 2$_1$/*n* 1			*P*1 2$_1$/*n* 1 (14)
h + *k*	*h*	*k*	*C*1–1	***C*121** (5)	***C*1*m*1** (8)	***C*1 2/*m* 1** (12)
h + *k*	*h*, *l*	*k*	*C*1*c*1		***C*1*c*1** (9)	***C*1 2/*c* 1** (15)
k + *l*	*l*	*k*	*A*1–1	*A*121 (5)	*A*1*m*1 (8)	*A*1 2/*m* 1 (12)
k + *l*	*h*, *l*	*k*	*A*1*n*1		*A*1*n*1 (9)	*A*1 2/*n* 1 (15)
h + *k* + *l*	*h* + *l*	*k*	*I*1–1	*I*121 (5)	*I*1*m*1 (8)	*I*1 2/*m* 1 (12)
h + *k* + *l*	*h*, *l*	*k*	*I*1*a*1		*I*1*a*1 (9)	*I*1 2/*a* 1 (15)

Unique axis *c*				Laue class 1 1 2/*m*		
Reflection conditions				Point group		
hkl 0*kl* *h*0*l*	*hk*0 *h*00 0*k*0	00*l*	Extinction symbol	2	*m*	2/*m*
			*P*11–	*P*112 (3)	*P*11*m* (6)	*P*11 2/*m* (10)
		l	*P*112$_1$	*P*112$_1$ (4)		*P*11 2$_1$/*m* (11)
	h		*P*11*a*		*P*11*a* (7)	*P*11 2/*a* (13)
	h	*l*	*P*11 2$_1$/*a*			*P*11 2$_1$/*a* (14)
	k		*P*11*b*		*P*11*b* (7)	*P*11 2/*b* (13)
	k	*l*	*P*11 2$_1$/*b*			*P*11 2$_1$/*b* (14)
	h + *k*		*P*11*n*		*P*11*n* (7)	*P*11 2/*n* (13)
	h + *k*	*l*	*P*11 2$_1$/*n*			*P*11 2$_1$/*n* (14)
h + *l*	*h*	*l*	*B*11–	*B*112 (5)	*B*11*m* (8)	*B*11 2/*m* (12)
h + *l*	*h*, *k*	*l*	*B*11*n*		*B*11*n* (9)	*B*11 2/*n* (15)
k + *l*	*k*	*l*	*A*11–	*A*112 (5)	*A*11*m* (8)	*A*11 2/*m* (12)
k + *l*	*h*, *k*	*l*	*A*11*a*		*A*11*a* (9)	*A*11 2/*a* (15)
h + *k* + *l*	*h* + *k*	*l*	*I*11–	*I*112 (5)	*I*11*m* (8)	*I*11 2/*m* (12)
h + *k* + *l*	*h*, *k*	*l*	*I*11*b*		*I*11*b* (9)	*I*11 2/*b* (15)

(3) *Incorrect assignment of the Laue symmetry*

This may be caused by pseudo-symmetry or by 'diffraction enhancement'. A crystal with pseudo-symmetry shows small deviations from a certain symmetry, and careful inspection of the diffraction pattern is necessary to determine the correct Laue class. In the case of diffraction enhancement, the symmetry of the diffraction pattern is higher than the Laue symmetry of the crystal. Structure types showing this phenomenon are rare and have to fulfil specified conditions. For further discussions and references, see Perez-Mato & Iglesias (1977).

3.1.5. Diffraction symbols and possible space groups

Table 3.1.4.1 contains 219 extinction symbols which, when combined with the Laue classes, lead to 242 different diffraction symbols. If, however, for the monoclinic and orthorhombic systems

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

MONOCLINIC, Laue class $2/m$ (*cont.*)

Unique axis *a*				Laue class $2/m$ 1 1		
Reflection conditions				Point group		
hkl *h*0*l* *hk*0	0*kl* 0*k*0 00*l*	*h*00	Extinction symbol	2	*m*	$2/m$
			P–11	*P*211 (3)	*Pm*11 (6)	$P2/m$ 11 (10)
		h	$P2_1 11$	$P2_1 11$ (4)		$P2_1/m$ 11 (11)
	k		*Pb*11		*Pb*11 (7)	$P2/b$ 11 (13)
	k	*h*	$P2_1/b$ 11			$P2_1/b$ 11 (14)
	l		*Pc*11		*Pc*11 (7)	$P2/c$ 11 (13)
	l	*h*	$P2_1/c$ 11			$P2_1/c$ 11 (14)
	$k+l$		*Pn*11		*Pn*11 (7)	$P2/n$ 11 (13)
	$k+l$	*h*	$P2_1/n$ 11			$P2_1/n$ 11 (14)
$h+k$	*k*	*h*	*C*–11	*C*211 (5)	*Cm*11 (8)	$C2/m$ 11 (12)
$h+k$	*k*, *l*	*h*	*Cn*11		*Cn*11 (9)	$C2/n$ 11 (15)
$h+l$	*l*	*h*	*B*–11	*B*211 (5)	*Bm*11 (8)	$B2/m$ 11 (12)
$h+l$	*k*, *l*	*h*	*Bb*11		*Bb*11 (9)	$B2/b$ 11 (15)
$h+k+l$	$k+l$	*h*	*I*–11	*I*211 (5)	*Im*11 (8)	$I2/m$ 11 (12)
$h+k+l$	*k*, *l*	*h*	*Ic*11		*Ic*11 (9)	$I2/c$ 11 (15)

ORTHORHOMBIC, Laue class *mmm* ($2/m$ $2/m$ $2/m$)

In this table, the symbol *e* in the space-group symbol represents the two glide planes given between parentheses in the corresponding extinction symbol. Only for one of the two cases does a bold printed symbol correspond with the standard symbol.

Reflection conditions								Laue class *mmm* ($2/m$ $2/m$ $2/m$)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
							P− − −	**P222** (16)	**Pmm2** (25)	**Pmmm** (47)
									*Pm*2*m* (25)	
									*P*2*mm* (25)	
						l	$P{-}{-}2_1$	**$P222_1$** (17)		
					k		$P{-}2_1{-}$	$P22_12$ (17)		
					k	*l*	$P{-}2_12_1$	$P22_12_1$ (18)		
				h			$P2_1{-}{-}$	$P2_122$ (17)		
				h		*l*	$P2_1{-}2_1$	$P2_122_1$ (18)		
				h	*k*		$P2_12_1{-}$	**$P2_12_12$** (18)		
				h	*k*	*l*	$P2_12_12_1$	**$P2_12_12_1$** (19)		
			h	*h*			*P*− −*a*		*Pm*2*a* (28)	
									$P2_1ma$ (26)	**Pmma** (51)
			k		*k*		*P*− −*b*		$Pm2_1b$ (26)	
									*P*2*mb* (28)	*Pmmb* (51)
			$h+k$	*h*	*k*		*P*− −*n*		$Pm2_1n$ (31)	
									$P2_1mn$ (31)	**Pmmn** (59)
		h		*h*			*P*−*a*−		**Pma2** (28)	*Pmam* (51)
									$P2_1am$ (26)	
		h	*h*	*h*			*P*−*aa*		*P*2*aa* (27)	*Pmaa* (49)
		h	*k*	*h*	*k*		*P*−*ab*		$P2_1ab$ (29)	*Pmab* (57)
		h	$h+k$	*h*	*k*		*P*−*an*		*P*2*an* (30)	*Pman* (53)
		l				*l*	*P*−*c*−		**$Pmc2_1$** (26)	
									*P*2*cm* (28)	*Pmcm* (51)
		l	*h*	*h*		*l*	*P*−*ca*		$P2_1ca$ (29)	*Pmca* (57)
		l	*k*		*k*	*l*	*P*−*cb*		*P*2*cb* (32)	*Pmcb* (55)
		l	$h+k$	*h*	*k*	*l*	*P*−*cn*		$P2_1cn$ (33)	*Pmcn* (62)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
		$h+l$		h		l	*P*–*n*–		$\mathbf{Pmn2_1}$ (31)	
									$P2_1nm$ (31)	*Pmnm* (59)
		$h+l$	h	h		l	*P*–*na*		*P*2*na* (30)	***Pmna*** (53)
		$h+l$	k	h	k	l	*P*–*nb*		$P2_1nb$ (33)	*Pmnb* (62)
		$h+l$	$h+k$	h	k	l	*P*–*nn*		*P*2*nn* (34)	*Pmnn* (58)
	k				k		*Pb*– –		*Pbm*2 (28)	
									$Pb2_1m$ (26)	*Pbmm* (51)
	k		h	h	k		*Pb*–*a*		$Pb2_1a$ (29)	*Pbma* (57)
	k		k		k		*Pb*–*b*		*Pb*2*b* (27)	*Pbmb* (49)
	k		$h+k$	h	k		*Pb*–*n*		*Pb*2*n* (30)	*Pbmn* (53)
	k	h		h	k		*Pba*–		***Pba*2** (32)	***Pbam*** (55)
	k	h	h	h	k		*Pbaa*			*Pbaa* (54)
	k	h	k	h	k		*Pbab*			*Pbab* (54)
	k	h	$h+k$	h	k		*Pban*			***Pban*** (50)
	k	l			k	l	*Pbc*–		$Pbc2_1$ (29)	***Pbcm*** (57)
	k	l	h	h	k	l	*Pbca*			***Pbca*** (61)
	k	l	k		k	l	*Pbcb*			*Pbcb* (54)
	k	l	$h+k$	h	k	l	*Pbcn*			***Pbcn*** (60)
	k	$h+l$		h	k	l	*Pbn*–		$Pbn2_1$ (33)	*Pbnm* (62)
	k	$h+l$	h	h	k	l	*Pbna*			*Pbna* (60)
	k	$h+l$	k	h	k	l	*Pbnb*			*Pbnb* (56)
	k	$h+l$	$h+k$	h	k	l	*Pbnn*			*Pbnn* (52)
	l					l	*Pc*– –		$Pcm2_1$ (26)	
									*Pc*2*m* (28)	*Pcmm* (51)
	l		h	h		l	*Pc*–*a*		*Pc*2*a* (32)	*Pcma* (55)
	l		k		k	l	*Pc*–*b*		$Pc2_1b$ (29)	*Pcmb* (57)
	l		$h+k$	h	k	l	*Pc*–*n*		$Pc2_1n$ (33)	*Pcmn* (62)
	l	h		h		l	*Pca*–		$\mathbf{Pca2_1}$ (29)	*Pcam* (57)
	l	h	h	h		l	*Pcaa*			*Pcaa* (54)
	l	h	k	h	k	l	*Pcab*			*Pcab* (61)
	l	h	$h+k$	h	k	l	*Pcan*			*Pcan* (60)
	l	l				l	*Pcc*–		***Pcc*2** (27)	***Pccm*** (49)
	l	l	h	h		l	*Pcca*			***Pcca*** (54)
	l	l	k		k	l	*Pccb*			*Pccb* (54)
	l	l	$h+k$	h	k	l	*Pccn*			***Pccn*** (56)
	l	$h+l$		h		l	*Pcn* –		*Pcn*2 (30)	*Pcnm* (53)
	l	$h+l$	h	h		l	*Pcna*			*Pcna* (50)
	l	$h+l$	k	h	k	l	*Pcnb*			*Pcnb* (60)
	l	$h+l$	$h+k$	h	k	l	*Pcnn*			*Pcnn* (52)
	$k+l$				k	l	*Pn* – –		$Pnm2_1$ (31)	*Pnmm* (59)
									$Pn2_1m$ (31)	
	$k+l$		h	h	k	l	*Pn*–*a*		$Pn2_1a$ (33)	***Pnma*** (62)
	$k+l$		k		k	l	*Pn*–*b*		*Pn*2*b* (30)	*Pnmb* (53)
	$k+l$		$h+k$	h	k	l	*Pn*–*n*		*Pn*2*n* (34)	*Pnmn* (58)
	$k+l$	h		h	k	l	*Pna* –		$\mathbf{Pna2_1}$ (33)	*Pnam* (62)
	$k+l$	h	h	h	k	l	*Pnaa*			*Pnaa* (56)
	$k+l$	h	k	h	k	l	*Pnab*			*Pnab* (60)
	$k+l$	h	$h+k$	h	k	l	*Pnan*			*Pnan* (52)
	$k+l$	l			k	l	*Pnc* –		***Pnc*2** (30)	*Pncm* (53)
	$k+l$	l	h	h	k	l	*Pnca*			*Pnca* (60)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
	k + *l*	*l*	*k*		*k*	*l*	*Pncb*			*Pncb* (50)
	k + *l*	*l*	*h* + *k*	*h*	*k*	*l*	*Pncn*			*Pncn* (52)
	k + *l*	*h* + *l*		*h*	*k*	*l*	*Pnn* −		***Pnn*2** (34)	***Pnnm*** (58)
	k + *l*	*h* + *l*	*h*	*h*	*k*	*l*	*Pnna*			***Pnna*** (52)
	k + *l*	*h* + *l*	*k*	*h*	*k*	*l*	*Pnnb*			*Pnnb* (52)
	k + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pnnn*			***Pnnn*** (48)
h + *k*	*k*	*h*	*h* + *k*	*h*	*k*		*C* − − −	***C*222** (21)	***Cmm*2** (35)	***Cmmm*** (65)
									*Cm*2*m* (38)	
									*C*2*mm* (38)	
h + *k*	*k*	*h*	*h* + *k*	*h*	*k*	*l*	$C--2_1$	**$C222_1$** (20)		
h + *k*	*k*	*h*	*h*, *k*	*h*	*k*		*C*− −(*ab*)		*Cm*2*e* (39)	***Cmme*** (67)
									*C*2*me* (39)	
h + *k*	*k*	*h*, *l*	*h* + *k*	*h*	*k*	*l*	*C*−*c* −		**$Cmc2_1$** (36)	***Cmcm*** (63)
									*C*2*cm* (40)	
h + *k*	*k*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*C*−*c*(*ab*)		*C*2*ce* (41)	***Cmce*** (64)
h + *k*	*k*, *l*	*h*	*h* + *k*	*h*	*k*	*l*	*Cc* − −		$Ccm2_1$ (36)	*Ccmm* (63)
									*Cc*2*m* (40)	
h + *k*	*k*, *l*	*h*	*h*, *k*	*h*	*k*	*l*	*Cc* −(*ab*)		*Cc*2*e* (41)	*Ccme* (64)
h + *k*	*k*, *l*	*h*, *l*	*h* + *k*	*h*	*k*	*l*	*Ccc* −		***Ccc*2** (37)	***Cccm*** (66)
h + *k*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*Ccc*(*ab*)			***Ccce*** (68)
h + *l*	*l*	*h* + *l*	*h*	*h*		*l*	*B* − − −	*B*222 (21)	*Bmm*2 (38)	*Bmmm* (65)
									*Bm*2*m* (35)	
									*B*2*mm* (38)	
h + *l*	*l*	*h* + *l*	*h*	*h*	*k*	*l*	$B{-}2_1{-}$	$B22_12$ (20)		
h + *l*	*l*	*h* + *l*	*h*, *k*	*h*	*k*	*l*	*B*− −*b*		$Bm2_1b$ (36)	*Bmmb* (63)
									*B*2*mb* (40)	
h + *l*	*l*	*h*, *l*	*h*	*h*		*l*	*B* −(*ac*)−		*Bme*2 (39)	*Bmem* (67)
									*B*2*em* (39)	
h + *l*	*l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*B* −(*ac*)*b*		*B*2*eb* (41)	*Bmeb* (64)
h + *l*	*k*, *l*	*h* + *l*	*h*	*h*	*k*	*l*	*Bb* − −		*Bbm*2 (40)	*Bbmm* (63)
									$Bb2_1m$ (36)	
h + *l*	*k*, *l*	*h* + *l*	*h*, *k*	*h*	*k*	*l*	*Bb*−*b*		*Bb*2*b* (37)	*Bbmb* (66)
h + *l*	*k*, *l*	*h*, *l*	*h*	*h*	*k*	*l*	*Bb*(*ac*)−		*Bbe*2 (41)	*Bbem* (64)
h + *l*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*Bb*(*ac*)*b*			*Bbeb* (68)
k + *l*	*k* + *l*	*l*	*k*		*k*	*l*	*A* − − −	*A*222 (21)	***Amm*2** (38)	*Ammm* (65)
									*Am*2*m* (38)	
									*A*2*mm* (35)	
k + *l*	*k* + *l*	*l*	*k*	*h*	*k*	*l*	$A2_1--$	$A2_122$ (20)		
k + *l*	*k* + *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*− −*a*		***Am*2*a*** (40)	*Amma* (63)
									$A2_1ma$ (36)	
k + *l*	*k* + *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*−*a* −		***Ama*2** (40)	*Amam* (63)
									$A2_1am$ (36)	
k + *l*	*k* + *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*−*aa*		*A*2*aa* (37)	*Amaa* (66)
k + *l*	*k*, *l*	*l*	*k*		*k*	*l*	*A*(*bc*)− −		***Aem*2** (39)	*Aemm* (67)
									*Ae*2*m* (39)	
k + *l*	*k*, *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)− *a*		*Ae*2*a* (41)	*Aema* (64)
k + *l*	*k*, *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*(*bc*)*a* −		***Aea*2** (41)	*Aeam* (64)
k + *l*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)*aa*			*Aeaa* (68)
h + *k* + *l*	*k* + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*I* − − −	[***I*222** (23) **$I2_12_12_1$**(24)]*	***Imm*2** (44)	***Immm*** (71)
									*Im*2*m* (44)	

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* ($2/m\ 2/m\ 2/m$) (*cont.*)

Reflection conditions								Laue class *mmm* ($2/m\ 2/m\ 2/m$)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
									*I*2*mm* (44)	
$h+k+l$	$k+l$	$h+l$	h, k	h	k	l	$I--(ab)$		*Im*2*a* (46)	***Imma*** (74)
									*I*2*mb* (46)	*Immb* (74)
$h+k+l$	$k+l$	h, l	$h+k$	h	k	l	$I-(ac)-$		***Ima*2** (46)	*Imam* (74)
									*I*2*cm* (46)	*lmcm* (74)
$h+k+l$	$k+l$	h, l	h, k	h	k	l	$I-cb$		*I*2*cb* (45)	*Imcb* (72)
$h+k+l$	k, l	$h+l$	$h+k$	h	k	l	$I(bc)--$		*Iem*2 (46)	*Iemm* (74)
									*Ie*2*m* (46)	
$h+k+l$	k, l	$h+l$	h, k	h	k	l	$Ic-a$		*Ic*2*a* (45)	*Icma* (72)
$h+k+l$	k, l	h, l	$h+k$	h	k	l	$Iba-$		***Iba*2** (45)	***Ibam*** (72)
$h+k+l$	k, l	h, l	h, k	h	k	l	$Ibca$			***Ibca*** (73)
										Icab (73)
$h+k, h+l, k+l$	k, l	h, l	h, k	h	k	l	$F---$	***F*222** (22)	***Fmm*2** (42)	***Fmmm*** (69)
									*Fm*2*m* (42)	
									*F*2*mm* (42)	
$h+k, h+l, k+l$	k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$F-dd$		*F*2*dd* (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$Fd-d$		*Fd*2*d* (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	h, k	$h=4n$	$k=4n$	$l=4n$	$Fdd-$		***Fdd*2** (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	$Fddd$			***Fddd*** (70)

* Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

TETRAGONAL, Laue classes $4/m$ and $4/mmm$

Reflection conditions							Extinction symbol	Laue class						
								$4/m$			$4/mmm$ ($4/m\ 2/m\ 2/m$)			
								Point group						
hkl	*hk*0	0*kl*	*hhl*	00*l*	0*k*0	*hh*0		4	$\bar{4}$	$4/m$	422	4*mm*	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
							$P---$	*P*4 (75)	$P\bar{4}$ (81)	$P4/m$ (83)	*P*422 (89)	*P*4*mm* (99)	$P\bar{4}2m$ (111)	$P4/mmm$ (123)
													$P\bar{4}m2$ (115)	
					k		$P-2_1-$				$P42_12$ (90)		$P\bar{4}2_1m$ (113)	
				l			$P4_2--$	$P4_2$ (77)		$P4_2/m$ (84)	$P4_222$ (93)			
				l	k		$P4_22_1-$				$P4_22_12$ (94)			
				$l=4n$			$P4_1--$	$\{P4_1$ (76), $P4_3$ (78)$\}$†			$\{P4_122$ (91), $P4_322$ (95)$\}$†			
				$l=4n$	k		$P4_12_1-$				$\{P4_12_12$ (92), $P4_32_12$ (96)$\}$†			
			l	l			$P--c$					$P4_2mc$ (105)	$P\bar{4}2c$ (112)	$P4_2/mmc$ (131)
			l	l	k		$P-2_1c$						$P\bar{4}2_1c$ (114)	
		k			k		$P-b-$					*P*4*bm* (100)	$P\bar{4}b2$ (117)	$P4/mbm$ (127)
		k	l	l	k		$P-bc$					$P4_2bc$ (106)		$P4_2/mbc$ (135)
		l		l			$P-c-$					$P4_2cm$ (101)	$P\bar{4}c2$ (116)	$P4_2/mcm$ (132)
		l	l	l			$P-cc$					*P*4*cc* (103)		$P4/mcc$ (124)
		$k+l$		l	k		$P-n-$					$P4_2nm$ (102)	$P\bar{4}n2$ (118)	$P4_2/mnm$ (136)
		$k+l$	l	l	k		$P-nc$					*P*4*nc* (104)		$P4/mnc$ (128)
	$h+k$				k		$Pn--$			$P4/n$ (85)				$P4/nmm$ (129)
	$h+k$			l	k		$P4_2/n--$			$P4_2/n$ (86)				
	$h+k$		l	l	k		$Pn-c$							$P4_2/nmc$ (137)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

TETRAGONAL, Laue classes $4/m$ and $4/mmm$ (*cont.*)

Reflection conditions							Extinction symbol	Laue class						
								$4/m$			$4/mmm$ ($4/m\ 2/m\ 2/m$)			
								Point group						
hkl	$hk0$	$0kl$	hhl	$00l$	$0k0$	$hh0$		4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
	$h+k$	k			k		$Pnb-$							$P4/nbm$ (125)
	$h+k$	k	l	l	k		$Pnbc$							$P4_2/nbc$ (133)
	$h+k$	l		l	k		$Pnc-$							$P4_2/ncm$ (138)
	$h+k$	l	l	l	k		$Pncc$							$P4/ncc$ (130)
	$h+k$	$k+l$		l	k		$Pnn-$							$P4_2/nnm$ (134)
	$h+k$	$k+l$	l	l	k		$Pnnc$							$P4/nnc$ (126)
$h+k+l$	$h+k$	$k+l$	l	l	k		$I---$	$I4$ (79)	$I\bar{4}$ (82)	$I4/m$ (87)	$I422$ (97)	$I4mm$ (107)	$I\bar{4}2m$ (121) $I\bar{4}m2$ (119)	$I4/mmm$ (139)
$h+k+l$	$h+k$	$k+l$	l	$l=4n$	k		$I4_1--$	$I4_1$ (80)			$I4_122$ (98)			
$h+k+l$	$h+k$	$k+l$	‡	$l=4n$	k	h	$I--d$					$I4_1md$ (109)	$I\bar{4}2d$ (122)	
$h+k+l$	$h+k$	k, l	l	l	k		$I-c-$					$I4cm$ (108)	$I\bar{4}c2$ (120)	$I4/mcm$ (140)
$h+k+l$	$h+k$	k, l	‡	$l=4n$	k	h	$I-cd$					$I4_1cd$ (110)		
$h+k+l$	h, k	$k+l$	l	$l=4n$	k		$I4_1/a--$			$I4_1/a$ (88)				
$h+k+l$	h, k	$k+l$	‡	$l=4n$	k	h	$Ia-d$							$I4_1/amd$ (141)
$h+k+l$	h, k	k, l	‡	$l=4n$	k	h	$Iacd$							$I4_1/acd$ (142)

† Pair of enantiomorphic space groups, *cf.* Section 3.1.5.
‡ Condition: $2h+l=4n$; l.

(as well as for the R space groups of the trigonal system), the different cell choices and settings of one space group are disregarded, 101 extinction symbols* and 122 diffraction symbols for the 230 space-group types result.

Only in 50 cases does a diffraction symbol uniquely identify just one space group, thus leaving 72 diffraction symbols that correspond to more than one space group. The 50 unique cases can be easily recognized in Table 3.1.4.1 because the line for the possible space groups in the particular Laue class contains just one entry.

The non-uniqueness of the space-group determination has two reasons:

(i) Friedel's rule, *i.e.* the effect that, with neglect of anomalous dispersion, the diffraction pattern contains an inversion centre, even if such a centre is not present in the crystal.

Example

A monoclinic crystal (with unique axis b) has the diffraction symbol $1\ 2/m\ 1P1c1$. Possible space groups are $P1c1$ (7) without an inversion centre, and $P12/c1$ (13) with an inversion centre. In both cases, the diffraction pattern has the Laue symmetry $1\ 2/m\ 1$.

One aspect of Friedel's rule is that the diffraction patterns are the same for two enantiomorphic space groups. Eleven diffraction symbols each correspond to a pair of enantiomorphic space groups. In Table 3.1.4.1, such pairs are grouped between braces. Either of the two space groups may be chosen for structure solution. If due to anomalous scattering Friedel's rule does not hold, at the refinement stage of structure determination it may be possible to determine the absolute structure and consequently the correct space group from the enantiomorphic pair.

(ii) The occurrence of four space groups in two 'special' pairs, each pair belonging to the same point group: $I222$ (23) & $I2_12_12_1$ (24) and $I23$ (197) & $I2_13$ (199). The two space groups of each pair differ in the location of the symmetry elements with respect to each other. In Table 3.1.4.1, these two special pairs are given in square brackets.

3.1.6. Space-group determination by additional methods

3.1.6.1. *Chemical information*

In some cases, chemical information determines whether or not the space group is centrosymmetric. For instance, all proteins crystallize in noncentrosymmetric space groups as they are constituted of L-amino acids only. Less certain indications may be obtained by considering the number of molecules per cell and the possible space-group symmetry. For instance, if experiment shows that there are two molecules of formula $A_\alpha B_\beta$ per cell in either space group $P2_1$ or $P2_1/m$ and if the molecule $A_\alpha B_\beta$ cannot possibly have either a mirror plane or an inversion centre, then there is a strong indication that the correct space group is $P2_1$. Crystallization of $A_\alpha B_\beta$ in $P2_1/m$ with random disorder of the molecules cannot be excluded, however. In a similar way, multiplicities of Wyckoff positions and the number of formula units per cell may be used to distinguish between space groups.

* The increase from 97 (*IT*, 1952) to 101 extinction symbols is due to the separate treatment of the trigonal and hexagonal crystal systems in Table 3.1.4.1, in contradistinction to *IT* (1952), Table 4.4.3, where they were treated together. In *IT* (1969), diffraction symbols were listed by Laue classes and thus the number of extinction symbols is the same as that of diffraction symbols, namely 122.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

TRIGONAL, Laue classes $\bar{3}$ and $\bar{3}m$

Reflection conditions				Extinction symbol	Laue class							
					$\bar{3}$		$\bar{3}m1$ ($\bar{3}$ $2/m$ 1) $\bar{3}m$			$\bar{3}1m$ ($\bar{3}$ 1 $2/m$)		
Hexagonal axes					Point group							
$hkil$	$h\bar{h}0l$	$hh\overline{2h}l$	$000l$		3	$\bar{3}$	321 32	$3m1$ $3m$	$\bar{3}m1$ $\bar{3}m$	312	$31m$	$\bar{3}1m$
				$P---$	P3 (143)	P$\bar{3}$ (147)	P321 (150)	P3m1 (156)	P$\bar{3}$m1 (164)	P312 (149)	P31m (157)	P$\bar{3}$1m (162)
			$l=3n$	$P3_1--$	{$P3_1$(144), $P3_2$(145)} §		{$P3_121$ (152), $P3_221$ (154)} §			{$P3_112$ (151), $P3_212$ (153)} §		
		l	l	$P--c$							P31c (159)	P$\bar{3}$1c (163)
	l		l	$P-c-$				P3cl (158)	P$\bar{3}$c1 (165)			
$-h+k+l=3n$	$h+l=3n$	$l=3n$	$l=3n$	R(obv)$--$ ¶	R3 (146)	R$\bar{3}$ (148)	R32 (155)	R3m (160)	R$\bar{3}$m (166)			
$-h+k+l=3n$	$h+l=3n$; l	$l=3n$	$l=6n$	R(obv)$-$ c				R3c (161)	R$\bar{3}$c (167)			
$h-k+l=3n$	$-h+l=3n$	$l=3n$	$l=3n$	R(rev)$--$	R3 (146)	R$\bar{3}$ (148)	R32 (155)	R3m (160)	R$\bar{3}$m (166)			
$h-k+l=3n$	$-h+l=3n$; l	$l=3n$	$l=6n$	R(rev)$-$ c				R3c (161)	R$\bar{3}$c (167)			

Rhombohedral axes				Extinction symbol	Point group				
hkl		hhl	hhh		3	$\bar{3}$	32	$3m$	$\bar{3}m$
				$R--$	$R3$(146)	$R\bar{3}$ (148)	$R32$ (155)	$R3m$ (160)	$R\bar{3}m$ (166)
		l	h	$R-c$				$R3c$ (161)	$R\bar{3}c$ (167)

§ Pair of enantiomorphic space groups; *cf.* Section 3.1.5.
¶ For obverse and reverse settings *cf.* Section 1.2.1. The obverse setting is standard in these tables.
The transformation reverse → obverse is given by **a**(obv.) = −**a**(rev.), **b**(obv.) = −**b**(rev.), **c**(obv.) = **c**(rev.).

HEXAGONAL, Laue classes $6/m$ and $6/mmm$

Reflection conditions			Extinction symbol	Laue class						
				$6/m$			$6/mmm$ ($6/m$ $2/m$ $2/m$)			
				Point group						
$h\bar{h}0l$	$hh\overline{2h}l$	$000l$		6	$\bar{6}$	$6/m$	622	$6mm$	$\bar{6}2m$ $\bar{6}m2$	$6/mmm$
			$P---$	$P6$ (168)	$P\bar{6}$ (174)	$P6/m$ (175)	$P622$ (177)	$P6mm$ (183)	$P\bar{6}2m$ (189) $P\bar{6}m2$ (187)	$P6/mmm$ (191)
		l	$P6_3--$	$P6_3$ (173)		$P6_3/m$ (176)	$P6_322$ (182)			
		$l=3n$	$P6_2--$	{$P6_2$ (171), $P6_4$ (172)} **			{$P6_222$ (180), $P6_422$ (181)} **			
		$l=6n$	$P6_1--$	{$P6_1$ (169), $P6_5$ (170)} **			{$P6_122$ (178), $P6_522$ (179)} **			
	l	l	$P--c$					$P6_3mc$ (186)	$P\bar{6}2c$ (190)	$P6_3/mmc$ (194)
l		l	$P-c-$					$P6_3cm$ (185)	$P\bar{6}c2$ (188)	$P6_3/mcm$ (193)
l	l	l	$P-cc$					$P6cc$ (184)		$P6/mcc$ (192)

** Pair of enantiomorphic space groups, *cf.* Section 3.1.5.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

CUBIC, Laue classes $m\bar{3}$ and $m\bar{3}m$

Reflection conditions (Indices are permutable, apart from space group No. 205) ††				Extinction symbol	Laue class: $m\bar{3}$ $(2/m\ \bar{3})$		Laue class: $m\bar{3}m$ $(4/m\ \bar{3}\ 2/m)$		
					Point group				
hkl	0*kl*	*hhl*	00*l*		23	$m\bar{3}$	432	$\bar{4}3m$	$m\bar{3}m$
				$P---$	$P23$ (195)	$Pm\bar{3}$ (200)	$P432$ (207)	$P\bar{4}3m$ (215)	$Pm\bar{3}m$ (221)
			l	$\{P2_1--$, $P4_2--\}$	$P2_13$ (198)		$P4_232$ (208)		
			$l=4n$	$P4_1--$			$\{P4_132$ (213), $P4_332$ (212)$\}$‡‡		
		l	l	$P--n$				$P\bar{4}3n$ (218)	$Pm\bar{3}n$ (223)
	k††		l	$Pa--$		$Pa\bar{3}$ (205)			
	$k+l$		l	$Pn--$		$Pn\bar{3}$ (201)			$Pn\bar{3}m$ (224)
	$k+l$	l	l	$Pn-n$					$Pn\bar{3}n$ (222)
$h+k+l$	$k+l$	l	l	$I---$	$[I23$ (197), $I2_13$ (199)$]$§§	$Im\bar{3}$ (204)	$I432$ (211)	$I\bar{4}3m$ (217)	$Im\bar{3}m$ (229)
$h+k+l$	$k+l$	l	$l=4n$	$I4_1--$			$I4_132$ (214)		
$h+k+l$	$k+l$	$2h+l=4n, l$	$l=4n$	$I--d$				$I\bar{4}3d$ (220)	
$h+k+l$	k, l	l	l	$Ia--$		$Ia\bar{3}$ (206)			
$h+k+l$	k, l	$2h+l=4n, l$	$l=4n$	$Ia-d$					$Ia\bar{3}d$ (230)
$h+k, h+l, k+l$	k, l	$h+l$	l	$F---$	$F23$ (196)	$Fm\bar{3}$ (202)	$F432$ (209)	$F\bar{4}3m$ (216)	$Fm\bar{3}m$ (225)
$h+k, h+l, k+l$	k, l	$h+l$	$l=4n$	$F4_1--$			$F4_132$ (210)		
$h+k, h+l, k+l$	k, l	h, l	l	$F--c$				$F\bar{4}3c$ (219)	$Fm\bar{3}c$ (226)
$h+k, h+l, k+l$	$k+l=4n, k, l$	$h+l$	$l=4n$	$Fd--$		$Fd\bar{3}$ (203)			$Fd\bar{3}m$ (227)
$h+k, h+l, k+l$	$k+l=4n, k, l$	h, l	$l=4n$	$Fd-c$					$Fd\bar{3}c$ (228)

†† For No. 205, only cyclic permutations are permitted. Conditions are 0*kl*: $k=2n$; *h*0*l*: $l=2n$; *hk*0: $h=2n$.
‡‡ Pair of enantiomorphic space groups, *cf.* Section 3.1.5.
§§ Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

3.1.6.2. *Point-group determination by methods other than the use of X-ray diffraction*

This is discussed in Chapter 10.2. In favourable cases, suitably chosen methods can prove the absence of an inversion centre or a mirror plane.

3.1.6.3. *Study of X-ray intensity distributions*

X-ray data can give a strong clue to the presence or absence of an inversion centre if not only the symmetry of the diffraction pattern but also the distribution of the intensities of the reflection spots is taken into account. Methods have been developed by Wilson and others that involve a statistical examination of certain groups of reflections. For a textbook description, see Lipson & Cochran (1966) and Wilson (1970). In this way, the presence of an inversion centre in a three-dimensional structure or in certain projections can be tested. Usually it is difficult, however, to obtain reliable conclusions from projection data. The same applies to crystals possessing pseudo-symmetry, such as a centrosymmetric arrangement of heavy atoms in a noncentrosymmetric structure. Several computer programs performing the statistical analysis of the diffraction intensities are available.

3.1.6.4. *Consideration of maxima in Patterson syntheses*

The application of Patterson syntheses for space-group determination is described by Buerger (1950, 1959).

3.1.6.5. *Anomalous dispersion*

Friedel's rule, $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$, does not hold for noncentrosymmetric crystals containing atoms showing anomalous dispersion. The difference between these intensities becomes particularly strong when use is made of a wavelength near the resonance level (absorption edge) of a particular atom in the crystal. Synchrotron radiation, from which a wide variety of wavelengths can be chosen, may be used for this purpose. In such cases, the diffraction pattern reveals the symmetry of the actual point group of the crystal (including the orientation of the point group with respect to the lattice).

3.1.6.6. *Summary*

One or more of the methods discussed above may reveal whether or not the point group of the crystal has an inversion centre. With this information, in addition to the diffraction symbol, 192 space groups can be uniquely identified. The rest consist of the eleven pairs of enantiomorphic space groups, the two 'special pairs' and six further ambiguities: 3 in the orthorhombic system (Nos. 26 & 28, 35 & 38, 36 & 40), 2 in the tetragonal system (Nos. 111 & 115, 119 & 121), and 1 in the hexagonal system (Nos. 187 & 189). If not only the point group but also its orientation with respect to the lattice can be determined, the six ambiguities can be resolved. This implies that 204 space groups can be uniquely identified, the only exceptions being the eleven pairs of enantiomorphic space groups and the two 'special pairs'.

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