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	Point group $\bar{1}$
None	$P-$	$P1$(1)	$P\bar{1}$ (2)

MONOCLINIC, Laue class $2/m$

Unique axis b — Laue class $1\ 2/m\ 1$

Reflection conditions hkl $0kl$ $hk0$	Reflection conditions $h0l$ $h00$ $00l$	Reflection conditions $0k0$	Extinction symbol	Point group 2	Point group m	Point group $2/m$
			$P1-1$	**$P121$** (3)	**$P1m1$** (6)	**$P1\ 2/m\ 1$** (10)
		k	$P12_11$	**$P12_11$** (4)		**$P1\ 2_1/m\ 1$** (11)
	h		$P1a1$		$P1a1$ (7)	$P1\ 2/a\ 1$ (13)
	h	k	$P1\ 2_1/a\ 1$			$P1\ 2_1/a\ 1$ (14)
	l		$P1c1$		**$P1c1$** (7)	**$P1\ 2/c\ 1$** (13)
	l	k	$P1\ 2_1/c\ 1$			**$P1\ 2_1/c\ 1$** (14)
	$h+l$		$P1n1$		$P1n1$ (7)	$P1\ 2/n\ 1$ (13)
	$h+l$	k	$P1\ 2_1/n\ 1$			$P1\ 2_1/n\ 1$ (14)
$h+k$	h	k	$C1-1$	**$C121$** (5)	**$C1m1$** (8)	**$C1\ 2/m\ 1$** (12)
$h+k$	h, l	k	$C1c1$		**$C1c1$** (9)	**$C1\ 2/c\ 1$** (15)
$k+l$	l	k	$A1-1$	$A121$ (5)	$A1m1$ (8)	$A1\ 2/m\ 1$ (12)
$k+l$	h, l	k	$A1n1$		$A1n1$ (9)	$A1\ 2/n\ 1$ (15)
$h+k+l$	$h+l$	k	$I1-1$	$I121$ (5)	$I1m1$ (8)	$I1\ 2/m\ 1$ (12)
$h+k+l$	h, l	k	$I1a1$		$I1a1$ (9)	$I1\ 2/a\ 1$ (15)

Unique axis c — Laue class $1\ 1\ 2/m$

Reflection conditions hkl $0kl$ $h0l$	Reflection conditions $hk0$ $h00$ $0k0$	Reflection conditions $00l$	Extinction symbol	Point group 2	Point group m	Point group $2/m$
			$P11-$	$P112$ (3)	$P11m$ (6)	$P11\ 2/m$ (10)
		l	$P112_1$	$P112_1$ (4)		$P11\ 2_1/m$ (11)
	h		$P11a$		$P11a$ (7)	$P11\ 2/a$ (13)
	h	l	$P11\ 2_1/a$			$P11\ 2_1/a$ (14)
	k		$P11b$		$P11b$ (7)	$P11\ 2/b$ (13)
	k	l	$P11\ 2_1/b$			$P11\ 2_1/b$ (14)
	$h+k$		$P11n$		$P11n$ (7)	$P11\ 2/n$ (13)
	$h+k$	l	$P11\ 2_1/n$			$P11\ 2_1/n$ (14)
$h+l$	h	l	$B11-$	$B112$ (5)	$B11m$ (8)	$B11\ 2/m$ (12)
$h+l$	h, k	l	$B11n$		$B11n$ (9)	$B11\ 2/n$ (15)
$k+l$	k	l	$A11-$	$A112$ (5)	$A11m$ (8)	$A11\ 2/m$ (12)
$k+l$	h, k	l	$A11a$		$A11a$ (9)	$A11\ 2/a$ (15)
$h+k+l$	$h+k$	l	$I11-$	$I112$ (5)	$I11m$ (8)	$I11\ 2/m$ (12)
$h+k+l$	h, k	l	$I11b$		$I11b$ (9)	$I11\ 2/b$ (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	$P211$ (3)	$Pm11$ (6)	$P2/m$ 11 (10)
		h	$P2_111$	$P2_111$ (4)		$P2_1/m$ 11 (11)
	k		$Pb11$		$Pb11$ (7)	$P2/b$ 11 (13)
	k	*h*	$P2_1/b$ 11			$P2_1/b$ 11 (14)
	l		$Pc11$		$Pc11$ (7)	$P2/c$ 11 (13)
	l	*h*	$P2_1/c$ 11			$P2_1/c$ 11 (14)
	$k+l$		$Pn11$		$Pn11$ (7)	$P2/n$ 11 (13)
	$k+l$	*h*	$P2_1/n$ 11			$P2_1/n$ 11 (14)
$h+k$	*k*	*h*	C–11	$C211$ (5)	$Cm11$ (8)	$C2/m$ 11 (12)
$h+k$	*k*, *l*	*h*	$Cn11$		$Cn11$ (9)	$C2/n$ 11 (15)
$h+l$	*l*	*h*	B–11	$B211$ (5)	$Bm11$ (8)	$B2/m$ 11 (12)
$h+l$	*k*, *l*	*h*	$Bb11$		$Bb11$ (9)	$B2/b$ 11 (15)
$h+k+l$	$k+l$	*h*	I–11	$I211$ (5)	$Im11$ (8)	$I2/m$ 11 (12)
$h+k+l$	*k*, *l*	*h*	$Ic11$		$Ic11$ (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*
							$P---$	$\mathbf{P222}$ (16)	$\mathbf{Pmm2}$ (25)	$\mathbf{Pmmm}$ (47)
									$Pm2m$ (25)	
									$P2mm$ (25)	
						l	$P--2_1$	$\mathbf{P222_1}$ (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*		$P2_12_1-$	$\mathbf{P2_12_12}$ (18)		
				h	*k*	*l*	$P2_12_12_1$	$\mathbf{P2_12_12_1}$ (19)		
			h	*h*			$P--a$		$Pm2a$ (28)	
									$P2_1ma$ (26)	$\mathbf{Pmma}$ (51)
			k		*k*		$P--b$		$Pm2_1b$ (26)	
									$P2mb$ (28)	$Pmmb$ (51)
			$h+k$	*h*	*k*		$P--n$		$Pm2_1n$ (31)	
									$P2_1mn$ (31)	$\mathbf{Pmmn}$ (59)
		h		*h*			$P-a-$		$\mathbf{Pma2}$ (28)	$Pmam$ (51)
									$P2_1am$ (26)	
		h	*h*	*h*			$P-aa$		$P2aa$ (27)	$Pmaa$ (49)
		h	*k*	*h*	*k*		$P-ab$		$P2_1ab$ (29)	$Pmab$ (57)
		h	$h+k$	*h*	*k*		$P-an$		$P2an$ (30)	$Pman$ (53)
		l				*l*	$P-c-$		$\mathbf{Pmc2_1}$ (26)	
									$P2cm$ (28)	$Pmcm$ (51)
		l	*h*	*h*		*l*	$P-ca$		$P2_1ca$ (29)	$Pmca$ (57)
		l	*k*		*k*	*l*	$P-cb$		$P2cb$ (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*−		**$Pmn2_1$** (31)	
									$P2_1nm$ (31)	*Pmnm* (59)
		$h+l$	h	h		l	*P*−*na*		*P2na* (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*		*P2nn* (34)	*Pmnn* (58)
	k				k		*Pb*− −		*Pbm2* (28)	
									$Pb2_1m$ (26)	*Pbmm* (51)
	k		h	h	k		*Pb*−*a*		$Pb2_1a$ (29)	*Pbma* (57)
	k		k		k		*Pb*−*b*		*Pb2b* (27)	*Pbmb* (49)
	k		$h+k$	h	k		*Pb*−*n*		*Pb2n* (30)	*Pbmn* (53)
	k	h		h	k		*Pba*−		***Pba2*** (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)	
									Pc2m (28)	*Pcmm* (51)
	l		h	h		l	*Pc*−*a*		*Pc2a* (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*−		**$Pca2_1$** (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*−		***Pcc2*** (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* −		*Pcn2* (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*		*Pn2b* (30)	*Pnmb* (53)
	$k+l$		$h+k$	h	k	l	*Pn*−*n*		*Pn2n* (34)	*Pnmn* (58)
	$k+l$	h		h	k	l	*Pna* −		**$Pna2_1$** (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* −		***Pnc2*** (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	***C*222$_1$** (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* −		***Cmc*2$_1$** (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* − −		*Ccm*2_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−	*B*2$2_1$2 (20)		
h + *l*	*l*	*h* + *l*	*h*, *k*	*h*	*k*	*l*	*B*− −*b*		*Bm*2_1*b* (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_1*m* (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*	*A*2_1− −	*A*$2_1$22 (20)		
k + *l*	*k* + *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*− −*a*		***Am*2*a*** (40)	*Amma* (63)
									A2_1*ma* (36)	
k + *l*	*k* + *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*−*a* −		***Ama*2** (40)	*Amam* (63)
									A2_1*am* (36)	
k + *l*	*k* + *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*−*aa*		*A*2*aa* (37)	*Amaa* (66)
k + *l*	*k*, *l*	*l*	*k*		*k*	*l*	*A*(*bc*)− −		***Aem*2** (39)	*Aemm* (67)
									*Ae*2*m* (39)	
k + *l*	*k*, *l*	*l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)− *a*		*Ae*2*a* (41)	*Aema* (64)
k + *l*	*k*, *l*	*h*, *l*	*k*	*h*	*k*	*l*	*A*(*bc*)*a* −		***Aea*2** (41)	*Aeam* (64)
k + *l*	*k*, *l*	*h*, *l*	*h*, *k*	*h*	*k*	*l*	*A*(*bc*)*aa*			*Aeaa* (68)
h + *k* + *l*	*k* + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*I* − − −	[***I*222** (23) ***I*2$_1$2$_1$2$_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)	*Imcm* (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)	*P*4/*m* (83)	*P*422 (89)	*P*4*mm* (99)	$P\bar{4}2m$ (111)	*P*4/*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)			
				$l=4n$			$P4_1$− −	$\left\{\begin{matrix} P4_1\ (76) \\ P4_3\ (78) \end{matrix}\right\}$†			$\left\{\begin{matrix} P4_122\ (91) \\ P4_322\ (95) \end{matrix}\right\}$†			
				$l=4n$	k		$P4_12_1$−				$\left\{\begin{matrix} P4_12_12\ (92) \\ P4_32_12\ (96) \end{matrix}\right\}$†			
			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)	*P*4/*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)		*P*4/*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)		*P*4/*mnc* (128)
	$h+k$				k		*Pn* − −			*P*4/*n* (85)				*P*4/*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	*hk*0	0*kl*	*hhl*	00*l*	0*k*0	*hh*0		4	$\bar{4}$	$4/m$	422	4*mm*	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
	$h+k$	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)	$I4/mmm$ (139)
													$I\bar{4}m2$ (119)	
$h+k+l$	$h+k$	$k+l$	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)
			$l=3n$	$P3_1--$	$\left\{\begin{matrix} P3_1(144) \\ P3_2(145) \end{matrix}\right\}$§		$\left\{\begin{matrix} P3_121\ (152) \\ P3_221\ (154) \end{matrix}\right\}$§			$\left\{\begin{matrix} P3_112\ (151) \\ P3_212\ (153) \end{matrix}\right\}$§		
		l	l	$P--c$							$P31c$ (159)	$P\bar{3}1c$ (163)
	l		l	$P-c-$				$P3c1$ (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)			
		$l=3n$	$P6_2--$	$\left\{\begin{matrix} P6_2\ (171) \\ P6_4\ (172) \end{matrix}\right\}$**			$\left\{\begin{matrix} P6_222\ (180) \\ P6_422\ (181) \end{matrix}\right\}$**			
		$l=6n$	$P6_1--$	$\left\{\begin{matrix} P6_1\ (169) \\ P6_5\ (170) \end{matrix}\right\}$**			$\left\{\begin{matrix} P6_122\ (178) \\ P6_522\ (179) \end{matrix}\right\}$**			
	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				
					$m\bar{3}$ ($2/m\ \bar{3}$)		$m\bar{3}m$ ($4/m\ \bar{3}\ 2/m$)		
					Point group				
hkl	$0kl$	hhl	$00l$		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	$\left\{\begin{matrix} P2_1 - - \\ P4_2 - - \end{matrix}\right.$	$P2_13$ (198)		$P4_232$ (208)		
			$l = 4n$	$P4_1 - -$			$\left\{\begin{matrix} P4_132\ (213) \\ P4_332\ (212) \end{matrix}\right\}$ ‡‡		
		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	$I - - -$	$\left[\begin{matrix} I23\ (197) \\ I2_13\ (199) \end{matrix}\right]$ §§	$Im\bar{3}$ (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 $0kl$: $k = 2n$; $h0l$: $l = 2n$; $hk0$: $h = 2n$.
‡‡ 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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4.1. Introduction to the synoptic tables

BY E. F. BERTAUT

4.1.1. Introduction

The synoptic tables of this section comprise two features:

(i) Space-group symbols for various settings and choices of the unit cell. Changes of the basis vectors generally cause changes of the Hermann–Mauguin space-group symbol. These axis transformations involve not only permutations of axes, conserving the shape of the cell, but also transformations which lead to different cell shapes and even to multiple cells.

(ii) Extended Hermann–Mauguin space-group symbols, in addition to the short and full symbols. The occurrence of 'additional symmetry elements' (see below) led to the introduction of 'extended space-group symbols' in *IT* (1952); they are systematically developed in the present section. These additional symmetry elements are displayed in the space-group diagrams and are important for the tabulated '*Symmetry operations*'.

For each crystal system, the text starts with a historical note on the synoptic tables in the earlier editions of *International Tables** followed by a discussion of points (i) and (ii) above. Finally, those group–subgroup relations (*cf.* Section 8.3.3) are treated that can be recognized from the full and the extended Hermann–Mauguin space-group symbols. This applies mainly to the *translationengleiche* or *t* subgroups (type **I**, *cf.* Section 2.2.15) and to the *klassengleiche* or *k* subgroups of type **IIa**. For the *k* subgroups of types **IIb** and **IIc**, inspection of the synoptic Table 4.3.2.1 provides easy recognition of only those subgroups which originate from the decentring of certain multiple cells: *C* or *F* in the tetragonal system (Section 4.3.4), *R* and *H* in the trigonal and hexagonal systems (Section 4.3.5).

4.1.2. Additional symmetry elements

In space groups, 'due to periodicity', symmetry elements occur that are not recorded in the Hermann–Mauguin symbols. These *additional symmetry elements* are products of a symmetry translation T and a symmetry operation W. This product is TW and its geometrical representation is found in the space-group diagrams (*cf.* Sections 8.1.2 and 11.1.1).†

Two cases have to be distinguished:

(i) *Symmetry operations of the same nature*

The symmetry operations W and TW are of the *same nature* and only the locations of their symmetry elements differ. This occurs when the translation vector **t** is *perpendicular* to the symmetry element of W (symmetry plane or symmetry axis); it also holds when W is an *inversion* or a *rotoinversion* (see below).

Table 4.1.2.1 summarizes the symmetry elements, located at the origin, and the location of those 'additional symmetry elements' which are generated by periodicity in the *interior* of the unit cell. 'Additional' axes $\bar{3}$, 6, 6_1, 6_2, 6_3, 6_4, 6_5 do not occur. The first column of Table 4.1.2.1 specifies W, the second column the translation vector **t**, the third the location of the symmetry element of TW. The last column indicates space groups and plane groups with representative diagrams. Other orientations of the symmetry axes and symmetry planes can easily be derived from the table.

Example

Let W be a threefold rotation with Seitz symbol $(3/0,0,0)$ and axis along 0, 0, *z*. The product with the translation $\mathsf{T}(1,0,0)$, perpendicular to the axis, is $(3/1,0,0)$ and again is a threefold rotation, for $(3/1,0,0)^3 = (1/0,0,0)$; its location is $\frac{2}{3}, \frac{1}{3}, z$.

Table 4.1.2.1 also deals with certain powers W^p of symmetry operations W, namely with $p = 2$ for operations of order four and with $p = 2, 3, 4$ for operations of order six. These powers give rise to their own 'additional symmetry elements', as illustrated by the following list and by the example below (operations of order 2 or 3 obviously do not have to be considered).

W	$4, 4_2$	$4_1, 4_3$	$\bar{4}$	6	$\bar{6}$	$\bar{3}$	6_1	6_5	6_3	6_2	6_4
W^p	2	2_1	2	$3, 2$	$3, m$	$3, \bar{1}$	$3_1, 2_1$	$3_2, 2_1$	$3, 2_1$	$3_2, 2$	$3_1, 2$

Example

6_2 in 0, 0, *z*; the powers to be considered are

$$(6_2)^2 = 3_2; \quad (6_2)^3 = 2; \quad (6_2)^4 = (3_2)^2.$$

The axes 3_2 and 2 at 0, 0, *z* create additional symmetry elements:

$$3_2 \text{ at } \tfrac{1}{3}, \tfrac{2}{3}, z;\ \tfrac{2}{3}, \tfrac{1}{3}, z \quad \text{and} \quad 2 \text{ at } \tfrac{1}{2}, 0, z;\ 0, \tfrac{1}{2}, z;\ \tfrac{1}{2}, \tfrac{1}{2}, z.$$

If W is an inversion operation with its centre of symmetry at point *M*, the operation TW creates an additional centre at the endpoint of the translation vector $\frac{1}{2}\mathbf{t}$, drawn from *M* (*cf.* Table 4.1.2.1, where *M* is in $0,0,0$).

(ii) *Symmetry operations of different nature*

The symmetry operations W and TW are of a *different nature* and have different symbols, corresponding to rotation and screw axes, to mirror and glide planes, to screw axes of different nature, and to glide planes of different nature, respectively.‡

In this case, the translation vector **t** has a component *parallel* to the symmetry axis or symmetry plane of W. This parallel component determines the nature and the symbol of the additional symmetry element, whereas the normal component of **t** is responsible for its location, as explained in Section 11.1.1. If the normal component is zero, symmetry element and additional symmetry element coincide geometrically. Note that such additional symmetry elements with glide or screw components exist even in symmorphic space groups.

Integral and centring translations: In primitive lattices, only integral translations occur and Tables 4.1.2.1 and 4.1.2.2 are relevant. For centred lattices, Tables 4.1.2.1 and 4.1.2.2 remain valid for the integral translations, whereas Table 4.1.2.3 has to be considered for the centring translations, which cause further 'additional symmetry elements'.

4.1.2.1. *Integral translations*

Table 4.1.2.2 lists representative symmetry elements, corresponding to W, and their associated glide planes and screw axes, corresponding to TW. The upper part of the table contains the diagonal twofold axes and symmetry planes that appear as tertiary symmetry elements in tetragonal and cubic space groups and as

* *Comparison tables*, pp. 28–44, *IT* (1935); *Index of symbols of space groups*, pp. 542–553, *IT* (1952).

† W is represented by $(\boldsymbol{W}, \boldsymbol{w})$ where $\boldsymbol{W}$ is the matrix part, $\boldsymbol{w}$ the column part, referred to a conventional coordinate system. T is represented by $(\boldsymbol{I}, \boldsymbol{t})$ and TW by $(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})$.

‡ The location and nature (screw axis, glide plane) of these additional symmetry elements were listed in the space-group tables of *IT* (1935) under the heading *Weitere Symmetrieelemente*, but were suppressed in *IT* (1952).