International Tables for Crystallography (2006). Vol. B, Appendix 1.4.3, pp. 120–149.

Appendix 1.4.3.

Structure-factor tables

Table A1.4.3.1. *Plane groups*

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

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

Table A1.4.3.2. *Triclinic space groups*

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

$P1$ [No. 1]

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

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

hkl	A	B
All	2(ccc − css − scs − ssc)	0

Table A1.4.3.3. *Monoclinic space groups*

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

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

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

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

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

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

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

Table A1.4.3.4. *Orthorhombic space groups*

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

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

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

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

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

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

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

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

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

Table A1.4.3.5. *Tetragonal space groups*

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

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

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

Explicit trigonometric functions given in the table follow the convention

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

Conditions for vanishing symbols:

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

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

$P4$ [No. 75]

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

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

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

$P4_2$ [No. 77]

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

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

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

$I4$ [No. 79]

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

$I4_1$ [No. 80]

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

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

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

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

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

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

$P4/m$ [No. 83]

hkl	A	B
All	4[P(cc) − M(ss)]c(lz)	0

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

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

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

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

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

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

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

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

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

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

$I4/m$ [No. 87]

hkl	A	B
All	8[P(cc) − M(ss)]c(lz)	0

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

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

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

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

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

$P422$ [No. 89]

hkl	A	B
All	4P(cc)c(lz)	−4M(ss)s(lz)

$P42_12$ [No. 90]

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

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

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

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

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

$P4_222$ [No. 93]

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

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

$P4_22_12$ [No. 94]

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

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

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

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

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

$I422$ [No. 97]

hkl	A	B
All	8P(cc)c(lz)	−8M(ss)s(lz)

$I4_122$ [No. 98]

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

$P4mm$ [No. 99]

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

$P4bm$ [No. 100]

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

$P4_2cm$ [No. 101]

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

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

$P4_2nm$ [No. 102]

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

$P4cc$ [No. 103]

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

$P4nc$ [No. 104]

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

$P4_2mc$ [No. 105]

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

$P4_2bc$ [No. 106]

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

$I4mm$ [No. 107]

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

$I4cm$ [No. 108]

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

$I4_1md$ [No. 109]

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

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

$I4_1cd$ [No. 110]

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

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

hkl	A	B
All	4P(cc)c(lz)	−4P(ss)s(lz)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

hkl	A	B
All	8P(cc)c(lz)	−8P(ss)s(lz)

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

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

$P4/mmm$ [No. 123]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$P4/ncc$ [No. 130, Origin 2] ($B = 0$ for all h, k, l)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$I4/mmm$ [No. 139]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where

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

and the abbreviations

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

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

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

Conditons for vanishing symbols:

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

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

$P3$ [No. 143]

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

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

l	*A*	*B*
$3n$	as for $P3$ [No. 143]	
$3n + 1$	$c(p_1 + u_1) + c(p_2 + u_2) + c(p_3 + u_3)$	$s(p_1 + u_1) + s(p_2 + u_2) + s(p_3 + u_3)$
$3n + 2$	$c(p_1 + u_1) + c(p_2 + u_3) + c(p_3 + u_2)$	$s(p_1 + u_1) + s(p_2 + u_3) + s(p_3 + u_2)$

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

l	*A*, *B*
$3n$	as for $P3$ [No. 143]
$3n + 1$	as for $l = 3n + 2$ in $P3_1$ [No. 144]
$3n + 2$	as for $l = 3n + 1$ in $P3_1$ [No. 144]

$R3$ [No. 146] (rhombohedral axes)

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

$R3$ [No. 146] (hexagonal axes)

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

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

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

hkl	*A*	*B*
All	$2[\mathrm{C}(hki)\mathrm{c}(lz) - \mathrm{S}(hki)\mathrm{s}(lz)]$	0

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

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

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

hkl	*A*	*B*
All	$6[\mathrm{C}(hki)\mathrm{c}(lz) - \mathrm{S}(hki)\mathrm{s}(lz)]$	0

*P*312 [No. 149]

hkl	*A*	*B*
All	$\mathrm{PH(cc)c}(lz) - \mathrm{PH(ss)s}(lz)$	$\mathrm{MH(cc)s}(lz) + \mathrm{MH(ss)c}(lz)$

*P*321 [No. 150]

hkl	*A*	*B*
All	$\mathrm{PH(cc)c}(lz) - \mathrm{MH(ss)s}(lz)$	$\mathrm{PH(ss)c}(lz) + \mathrm{MH(cc)s}(lz)$

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

l	*A*	*B*
$3n$	as for *P*312 [No. 149]	
$3n+1$	$\mathrm{c}(p_1+u_1)+\mathrm{c}(p_2+u_2)+\mathrm{c}(p_3+u_3)+\mathrm{c}(q_1+u_2)$ $+\mathrm{c}(q_2+u_3)+\mathrm{c}(q_3+u_1)]$	$\mathrm{s}(p_1+u_1)+\mathrm{s}(p_2+u_2)+\mathrm{s}(p_3+u_3)-\mathrm{s}(q_1+u_2)$ $-\mathrm{s}(q_2+u_3)-\mathrm{s}(q_3+u_1)$
$3n+2$	$\mathrm{c}(p_1+u_1)+\mathrm{c}(p_2+u_3)+\mathrm{c}(p_3+u_2)+\mathrm{c}(q_1+u_3)$ $+\mathrm{c}(q_2+u_2)+\mathrm{c}(q_3+u_1)$	$\mathrm{s}(p_1+u_1)+\mathrm{s}(p_2+u_3)+\mathrm{s}(p_3+u_2)-\mathrm{s}(q_1+u_3)$ $-\mathrm{s}(q_2+u_2)-\mathrm{s}(q_3+u_1)$

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

l	*A*	*B*
$3n$	as for *P*321 [No. 150]	
$3n+1$	$\mathrm{c}(p_1+u_1)+\mathrm{c}(p_2+u_2)+\mathrm{c}(p_3+u_3)+\mathrm{c}(q_1-u_1)$ $+\mathrm{c}(q_2-u_2)+\mathrm{c}(q_3-u_3)$	$\mathrm{s}(p_1+u_1)+\mathrm{s}(p_2+u_2)+\mathrm{s}(p_3+u_3)+\mathrm{s}(q_1-u_1)$ $+\mathrm{s}(q_2-u_2)+\mathrm{s}(q_3-u_3)$
$3n+2$	$\mathrm{c}(p_1+u_1)+\mathrm{c}(p_2+u_3)+\mathrm{c}(p_3+u_2)+\mathrm{c}(q_1-u_1)$ $+\mathrm{c}(q_2-u_3)+\mathrm{c}(q_3-u_2)$	$\mathrm{s}(p_1+u_1)+\mathrm{s}(p_2+u_3)+\mathrm{s}(p_3+u_2)+\mathrm{s}(q_1-u_1)$ $+\mathrm{s}(q_2-u_3)+\mathrm{s}(q_3-u_2)$

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

l	*A*, *B*
$3n$	as for *P*312 [No. 149]
$3n+1$	as for $l = 3n+2$ in $P3_112$ [No. 151]
$3n+2$	as for $l = 3n+1$ in $P3_112$ [No. 151]

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

l	*A*, *B*
$3n$	as for *P*321 [No. 150]
$3n+1$	as for $l = 3n+2$ in $P3_121$ [No. 152]
$3n+2$	as for $l = 3n+1$ in $P3_121$ [No. 152]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

A
2[PH(cc)c(lz) − PH(ss)s(lz)]

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

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

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

A
2[PH(cc)c(lz) − MH(ss)s(lz)]

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

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

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

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

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

A
6[PH(cc)c(lz) − MH(ss)s(lz)]

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

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

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

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

$P6$ [No. 168]

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

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

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

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

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

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

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

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

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

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

$P6_3$ [No. 173]

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

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

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

$P6/m$ [No. 175]

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

$P6_3/m$ [No. 176]

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

$P622$ [No. 177]

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

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

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

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

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

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

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

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

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

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

$P6_322$ [No. 182]

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

$P6mm$ [No. 183]

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

$P6cc$ [No. 184]

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

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

$P6_3cm$ [No. 185]

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

$P6_3mc$ [No. 186]

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

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

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

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

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

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

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

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

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

$P6/mmm$ [No. 191]

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

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

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

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

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

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

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

Table A1.4.3.7. *Cubic space groups*

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

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

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

and

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

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

Conditions for vanishing symbols:

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

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

*P*23 [No. 195]

hkl	*A*	*B*
All	4Eccc	−4Esss

*F*23 [No. 196]

hkl	*A*	*B*
All	16Eccc	−16Esss

*I*23 [No. 197]

hkl	*A*	*B*
All	8Eccc	−8Esss

$P2_13$ [No. 198]

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

$I2_13$ [No. 199]

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

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

hkl	*A*	*B*
All	8Eccc	0

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

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

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

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

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

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

hkl	A	B
All	32Eccc	0

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

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

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

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

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

hkl	A	B
All	16Eccc	0

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

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

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

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

$P432$ [No. 207]

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

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

$P4_232$ [No. 208]

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

$F432$ [No. 209]

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

$F4_132$ [No. 210]

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

$I432$ [No. 211]

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

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

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

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

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

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

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

$I4_132$ [No. 214]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

hkl	A	B
All	8(Eccc + Occc)	0

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

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

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

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

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

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

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

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

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

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

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

hkl	A	B
All	32(Eccc + Occc)	0

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

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

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

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

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

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

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

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

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

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

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

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

hkl	A	B
All	16(Eccc + Occc)	0

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

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

references