International Tables for Crystallography (2010). Vol. B, Table A1.4.3.5, pp. 141–149.

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

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

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

Table A1.4.3.5 (*cont.*)

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

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

$P4/m$ [No. 83]

hkl	A	B
All	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	0

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

l	A
$2n$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$
$2n+1$	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$

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

$h+k$	A	B
$2n$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	0
$2n+1$	0	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$

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

h	k	A
$2n$	$2n$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$
$2n$	$2n+1$	$-4[\mathrm{P(cs)} + \mathrm{M(sc)}]\mathrm{s}(lz)$
$2n+1$	$2n$	$-4[\mathrm{M(cs)} + \mathrm{P(sc)}]\mathrm{s}(lz)$
$2n+1$	$2n+1$	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{c}(lz)$

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

$h+k+l$	A	B
$2n$	$4[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	0
$2n+1$	0	$4[\mathrm{M(cc)} - \mathrm{P(ss)}]\mathrm{s}(lz)$

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

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

$I4/m$ [No. 87]

hkl	A	B
All	$8[\mathrm{P(cc)} - \mathrm{M(ss)}]\mathrm{c}(lz)$	0

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

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

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

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

Table A1.4.3.5 (*cont.*)

$P422$ [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)

$P4_22_12$ [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)}

Table A1.4.3.5 (*cont.*)

*P*4*mm* [No. 99]

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

*P*4*bm* [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)

$P4_2nm$ [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)

*P*4*cc* [No. 103]

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

*P*4*nc* [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)

*I*4*mm* [No. 107]

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

*I*4*cm* [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 (*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
$2n$	$4P(cc)c(lz)$	$4M(cc)s(lz)$
$2n+1$	$-4M(ss)c(lz)$	$-4P(ss)s(lz)$

$I\bar{4}m2$ [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	$8P(cc)c(lz)$	$-8P(ss)s(lz)$

Table A1.4.3.5 (*cont.*)

$I\bar{4}2d$ [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)

$P4/nnc$ [No. 126, Origin 1]

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

$P4/nnc$ [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)

$P4/mbm$ [No. 127] (B = 0 for all h, k, l)

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

$P4/mnc$ [No. 128] (B = 0 for all h, k, l)

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

$P4/nmm$ [No. 129, Origin 1]

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

Table A1.4.3.5 (*cont.*)

$P4/nmm$ [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)

$P4/ncc$ [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)

$P4/ncc$ [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)

Table A1.4.3.5 (*cont.*)

$P4_2/nnm$ [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)

$P4_2/mbc$ [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

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

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

Table A1.4.3.5 (*cont.*)

$I4_1/amd$ [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)]

references