International Tables for Crystallography (2010). Vol. B, Table A1.4.3.6, pp. 150–155.

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 $\mathrm{c}(x)$ and $\mathrm{s}(x)$, respectively. All the symbols used in this table are repeated below. Most expressions are given in terms of

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

where

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

and the abbreviations

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

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

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

Conditons for vanishing symbols:

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

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	$\mathrm{C}(hki)\mathrm{c}(lz) - \mathrm{S}(hki)\mathrm{s}(lz)$	$\mathrm{C}(hki)\mathrm{s}(lz) + \mathrm{S}(hki)\mathrm{c}(lz)$

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

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

$P3_2$ [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	$\mathrm{c}(hx+ky+lz) + \mathrm{c}(kx+ly+hz) + \mathrm{c}(lx+hy+kz)$	$\mathrm{s}(hx+ky+lz) + \mathrm{s}(kx+ly+hz) + \mathrm{s}(lx+hy+kz)$

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

hkl	*A*	*B*
All	$3[\mathrm{C}(hki)\mathrm{c}(lz) - \mathrm{S}(hki)\mathrm{s}(lz)]$	$3[\mathrm{C}(hki)\mathrm{s}(lz) + \mathrm{S}(hki)\mathrm{c}(lz)]$

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

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

Table A1.4.3.6 (*cont.*)

$R\bar{3}$ [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

$P312$ [No. 149]

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

$P321$ [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 $P312$ [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 $P321$ [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 $P312$ [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 $P321$ [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]

$R32$ [No. 155] (rhombohedral axes)

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

$R32$ [No. 155] (hexagonal axes)

hkl	A	B
All	$3[\mathrm{PH(cc)c}(lz)-\mathrm{MH(ss)s}(lz)]$	$3[\mathrm{PH(ss)c}(lz)+\mathrm{MH(cc)s}(lz)]$

$P3m1$ [No. 156]

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

Table A1.4.3.6 (*cont.*)

*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*)]

$P\bar{3}1m$ [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*
2*n*	2[PH(cc)c(*lz*) − PH(ss)s(*lz*)]
2*n* + 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*
2*n*	2[PH(cc)c(*lz*) − MH(ss)s(*lz*)]
2*n* + 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)

Table A1.4.3.6 (*cont.*)

$R\bar{3}m$ [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)
$6n+4$	$2[c(p_1)c(u_1) + c(p_2)c(u_2) + c(p_3)c(u_3)]$	$2[c(p_1)s(u_1) + c(p_2)s(u_2) + c(p_3)s(u_3)]$
$6n+5$	$-2[s(p_1)s(u_1) + s(p_2)s(u_3) + s(p_3)s(u_2)]$	$2[s(p_1)c(u_1) + s(p_2)c(u_3) + s(p_3)c(u_2)]$

$P6_5$ [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)

Table A1.4.3.6 (*cont.*)

$P6/m$ [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	$2PH(cc)c(lz)$	$2MH(cc)s(lz)$

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

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

$P6_522$ [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	$2PH(cc)c(lz)$	$2PH(cc)s(lz)$

Table A1.4.3.6 (*cont.*)

$P6cc$ [No. 184]

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

$P6_3cm$ [No. 185]

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

$P6_3mc$ [No. 186]

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

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

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

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

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

references