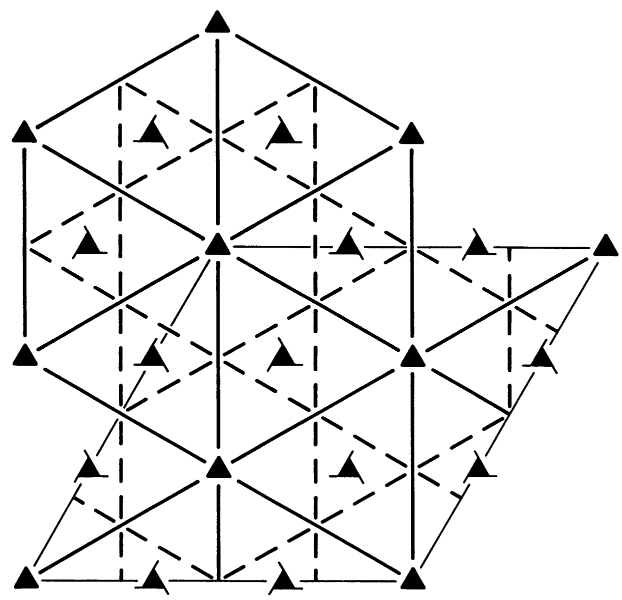
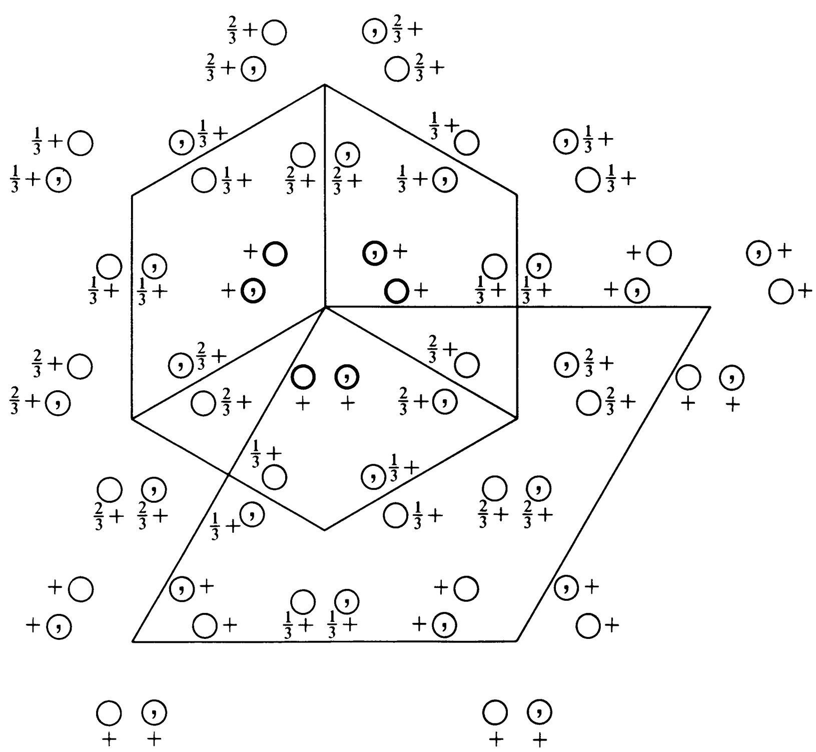
International Tables for Crystallography (2016). Vol. A, Space group 160, pp. 522–525.

$R3m$ $\quad C_{3v}^5$ $\quad 3m$ $\quad$ Trigonal

No. 160 $\quad R3m$ $\quad$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3m$

Asymmetric unit $\quad 0 \le x \le \frac{2}{3}; \quad 0 \le y \le \frac{2}{3}; \quad 0 \le z \le \frac{1}{3}; \quad x \le 2y; \quad y \le \min(1-x, 2x)$

Vertices $\quad 0,0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{3} \quad \frac{2}{3},\frac{1}{3},\frac{1}{3} \quad \frac{1}{3},\frac{2}{3},\frac{1}{3}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $m\ \ x,\bar{x},z$	(5) $m\ \ x,2x,z$	(6) $m\ \ 2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^{+}(0,0,\frac{1}{3})\ \ \frac{1}{3},\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{1}{3})\ \ \frac{1}{3},0,z$
(4) $g(\frac{1}{6},-\frac{1}{6},\frac{1}{3})\ \ x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{6},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{4},2x,z$	(6) $g(\frac{2}{3},\frac{1}{3},\frac{1}{3})\ \ 2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^{+}(0,0,\frac{2}{3})\ \ 0,\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{2}{3})\ \ \frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{6},\frac{1}{6},\frac{2}{3})\ \ x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{3},\frac{2}{3},\frac{2}{3})\ \ x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3})\ \ 2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\ \ (\frac{2}{3},\frac{1}{3},\frac{1}{3})+\ \ (\frac{1}{3},\frac{2}{3},\frac{2}{3})+$			Reflection conditions
						General:
18	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$	$hki0$: $-h+k=3n$
						$hh\overline{2h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$
						$000l$: $l=3n$
						$h\bar{h}00$: $h=3n$
						Special: no extra conditions
9	b	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
3	a	$3m$	$0,0,z$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

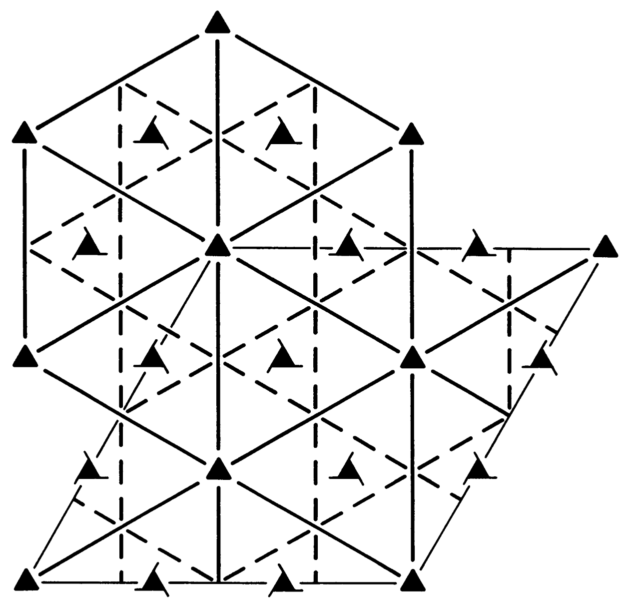
Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

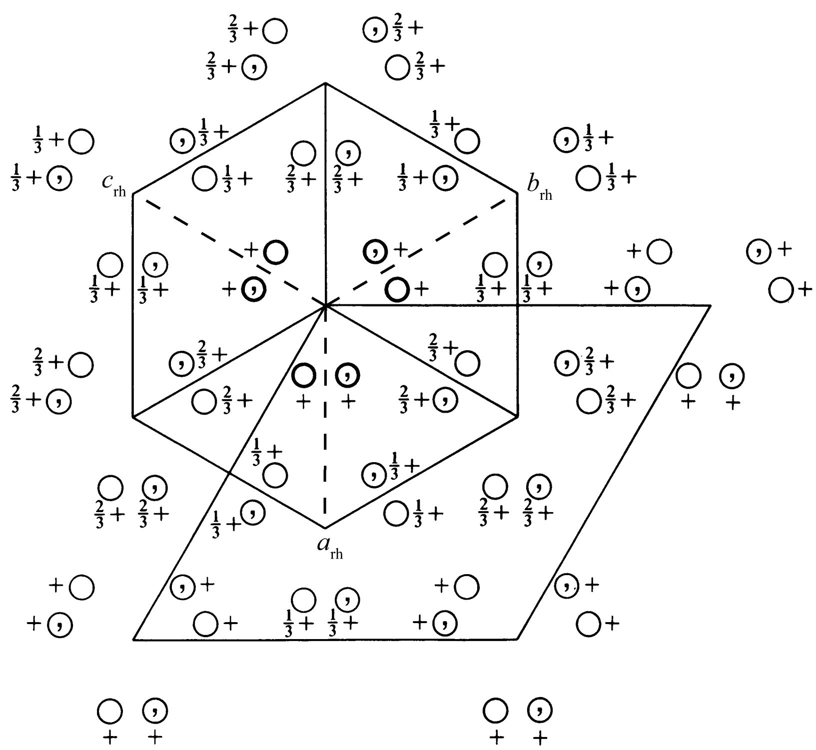
Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$R3m$ C_{3v}^{5} $3m$ Trigonal

No. 160 $R3m$ Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on $3m$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le 1$; $y \le x$; $z \le y$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $1,1,1$

Symmetry operations

(1) 1 (2) 3^{+} x,x,x (3) 3^{-} x,x,x
(4) m x,y,x (5) m x,x,z (6) m x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) z,y,x	(5) y,x,z	(6) x,z,y	
						Special: no extra conditions
3	b	$.m$	x,y,x	x,x,y	y,x,x	
1	a	$3m$	x,x,x			

Symmetry of special projections

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$