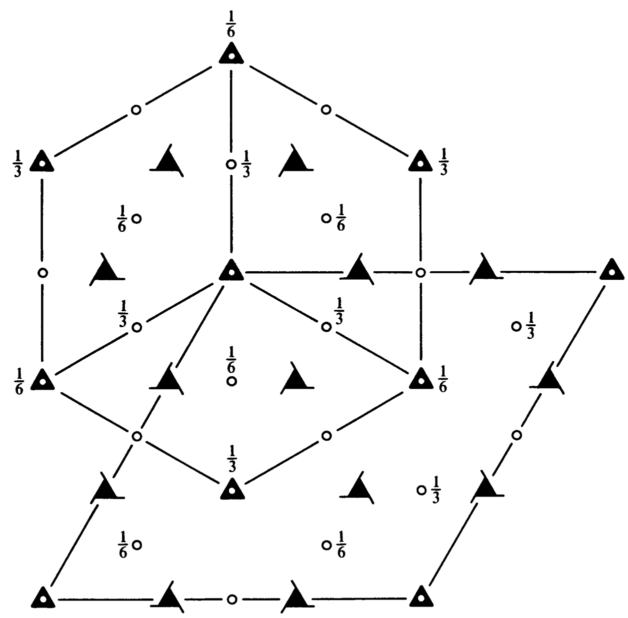
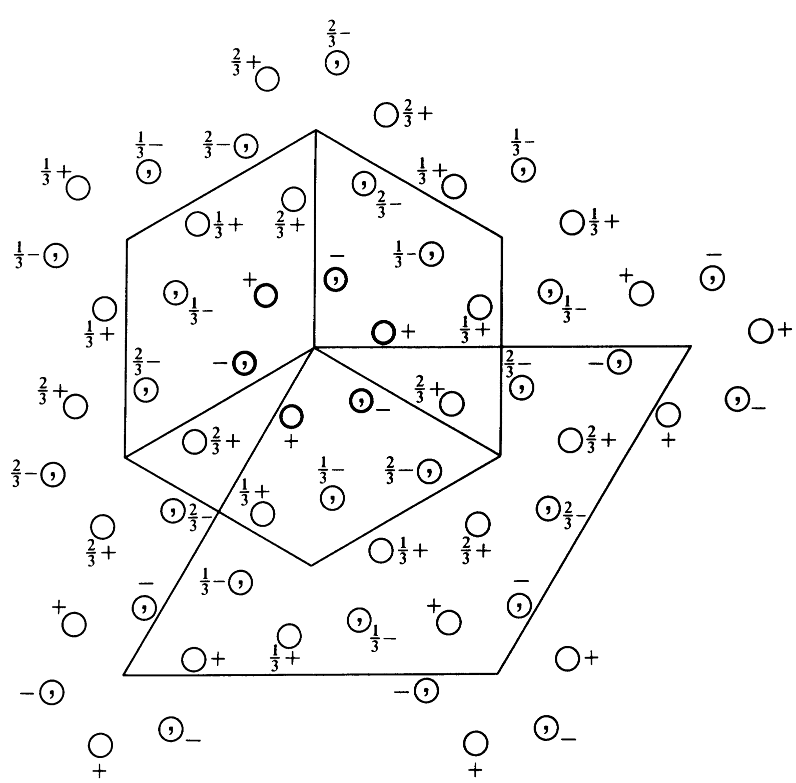
International Tables for Crystallography (2016). Vol. A, Space group 148, pp. 504–507.

$R\bar{3}$ C_{3i}^{2} $\bar{3}$ Trigonal

No. 148 $R\bar{3}$ Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin at centre ($\bar{3}$)

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

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

$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$

Symmetry operations

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

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

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) $\bar{1}\ \ \frac{1}{3},\frac{1}{6},\frac{1}{6}$	(5) $\bar{3}^{+}\ \frac{1}{3},-\frac{1}{3},z;\ \ \frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(6) $\bar{3}^{-}\ \frac{1}{3},\frac{2}{3},z;\ \ \frac{1}{3},\frac{2}{3},\frac{1}{6}$

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) $\bar{1}\ \ \frac{1}{6},\frac{1}{3},\frac{1}{3}$	(5) $\bar{3}^{+}\ \frac{2}{3},\frac{1}{3},z;\ \ \frac{2}{3},\frac{1}{3},\frac{1}{3}$	(6) $\bar{3}^{-}\ -\frac{1}{3},\frac{1}{3},z;\ \ -\frac{1}{3},\frac{1}{3},\frac{1}{3}$

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: $(0,0,0)+\quad(\frac{2}{3},\frac{1}{3},\frac{1}{3})+\quad(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ — Reflection conditions

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

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

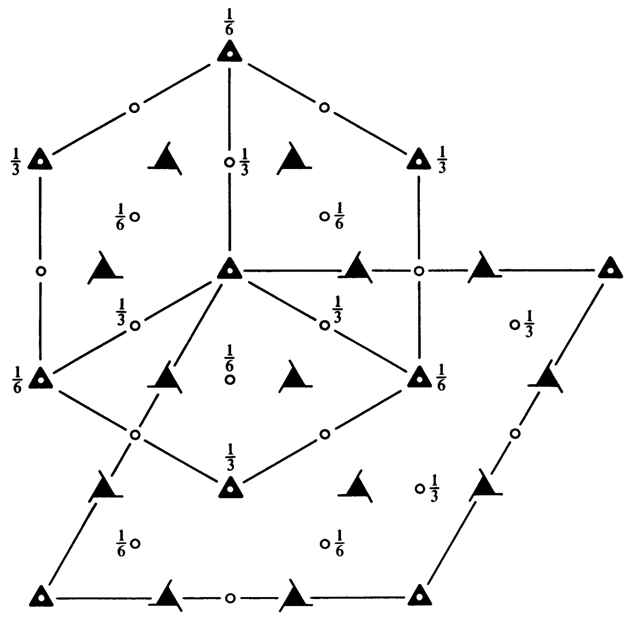
Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})\quad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

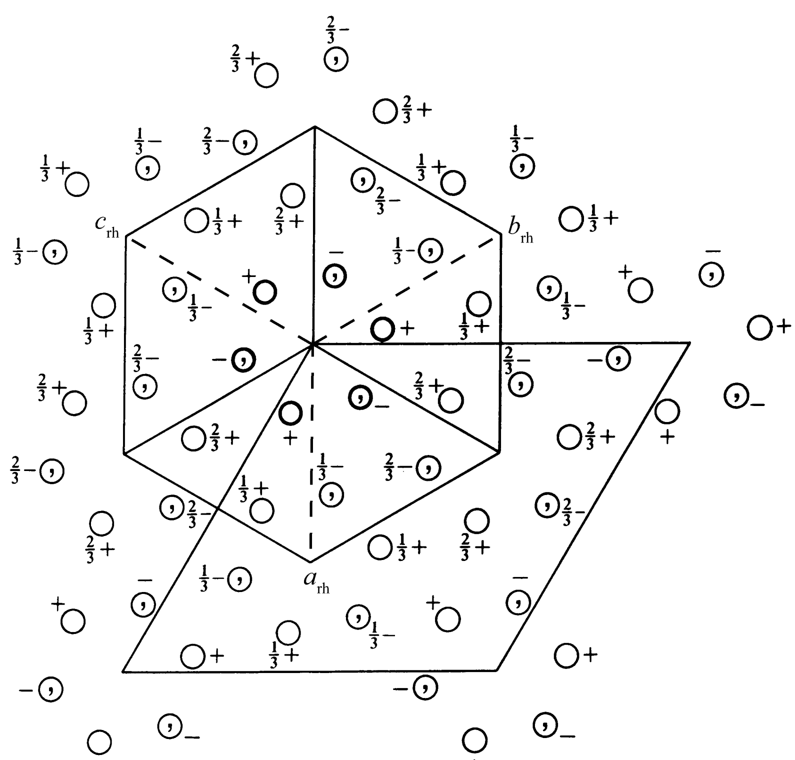
Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\quad \mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$R\bar{3}$ C_{3i}^2 $\bar{3}$ Trigonal

No. 148 $R\bar{3}$ Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin at centre ($\bar{3}$)

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

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

Symmetry operations

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

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	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $\bar{z},\bar{x},\bar{y}$	(6) $\bar{y},\bar{z},\bar{x}$	
						Special: no extra conditions
3	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	
3	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	
2	c	$3\,.$	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	b	$\bar{3}\,.$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	a	$\bar{3}\,.$	$0,0,0$			

Symmetry of special projections

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along $[1\bar{1}0]$ $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$