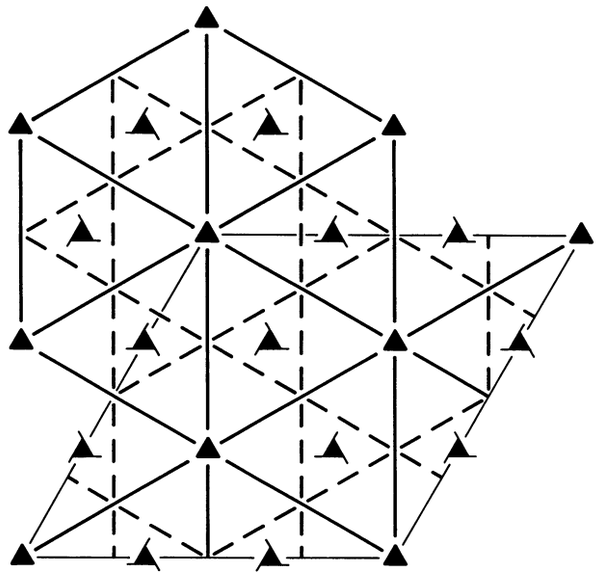
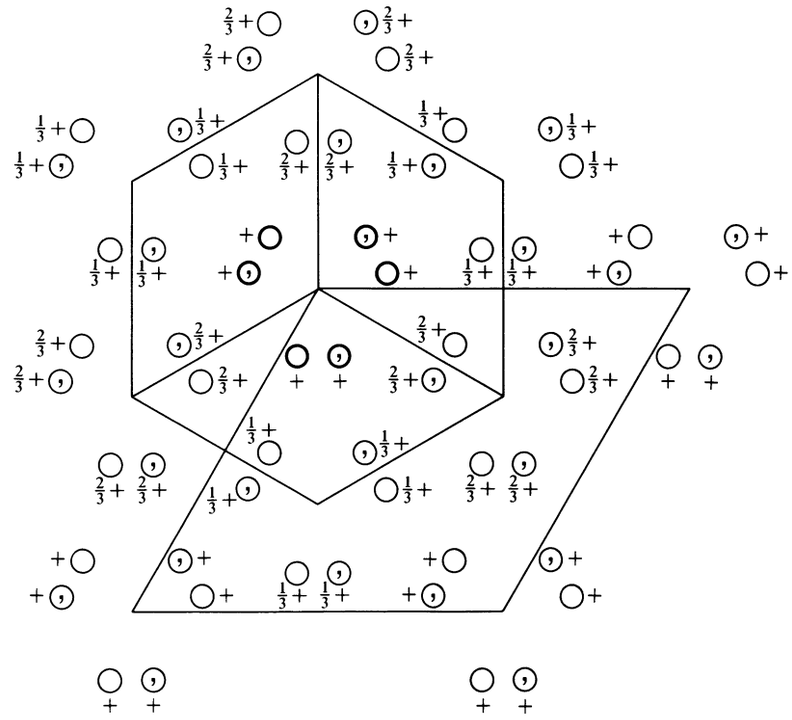
International Tables for Crystallography (2006). Vol. A, Space group 160, pp. 528–529.

$R3m$ $\quad C_{3v}^{5}$ $\quad 3m$ $\quad$ 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) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3})\ \ 2x-\frac{1}{2},x,z$

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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		
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$
9	b	$.\,m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$
3	a	$3\,m$	$0,0,z$		

Reflection conditions

General:

$hkil$: $-h+k+l=3n$
$hki0$: $-h+k=3n$
$hh\overline{2h}l$: $l=3n$
$h\bar{h}0l$: $h+l=3n$
$000l$: $l=3n$
$h\bar{h}00$: $h=3n$

Special: no extra conditions

Symmetry of special projections

Along [001] $p3\,1\,m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

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

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

Maximal non-isomorphic subgroups

I [2] $R3\,1$ ($R3$, 146) (1; 2; 3)+
{ [3] $R\,1\,m$ (Cm, 8) (1; 4)+
[3] $R\,1\,m$ (Cm, 8) (1; 5)+
[3] $R\,1\,m$ (Cm, 8) (1; 6)+

IIa [3] $P3\,m\,1$ (156) 1; 2; 3; 4; 5; 6

IIb [2] $R3\,c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (161)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3\,m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (160); [4] $R3\,m$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (160)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}m$ (166); [4] $P\bar{4}3\,m$ (215); [4] $F\bar{4}3\,m$ (216); [4] $I\bar{4}3\,m$ (217)

II [3] $P3\,1\,m$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (157)