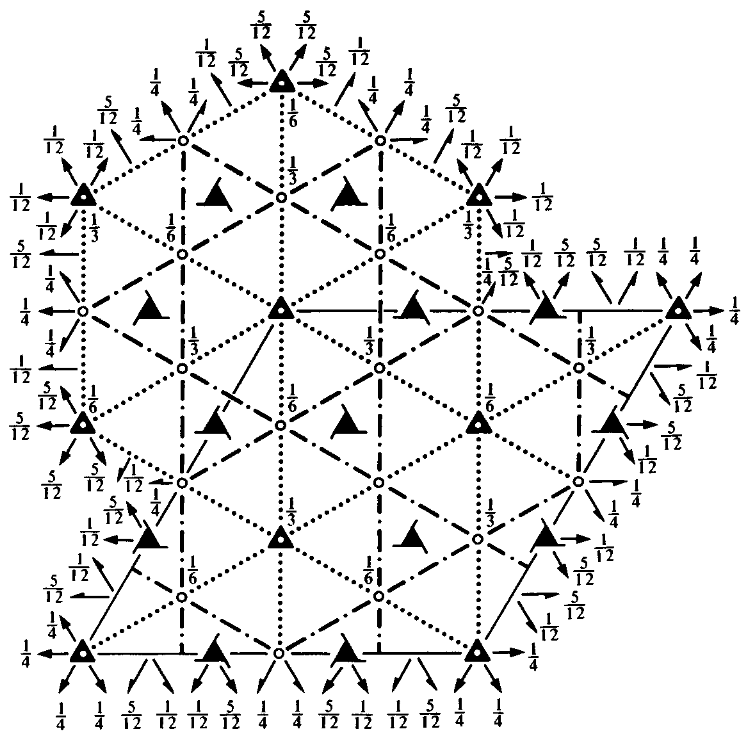
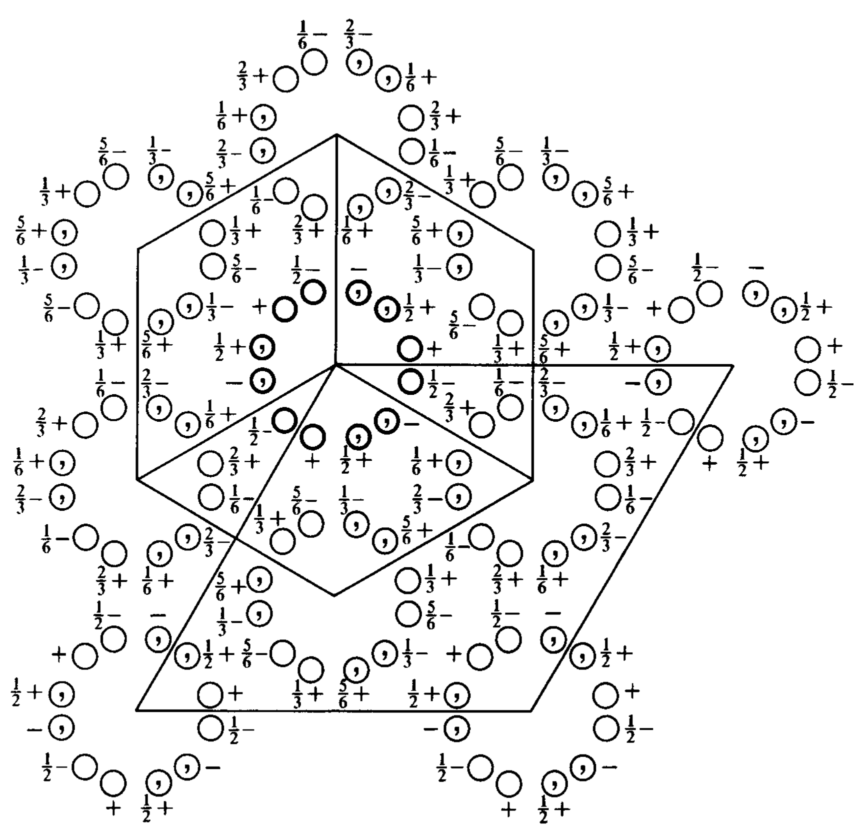
International Tables for Crystallography (2006). Vol. A, Space group 167, pp. 548–551.

$R\bar{3}c$ D_{3d}^{6} $\bar{3}m$ Trigonal

No. 167 $R\bar{3}2/c$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





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

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{12}$; $x \le (1+y)/2$; $y \le \min(1-x, (1+x)/2)$

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

$0,0,\frac{1}{12}$ $\frac{1}{2},0,\frac{1}{12}$ $\frac{2}{3},\frac{1}{3},\frac{1}{12}$ $\frac{1}{3},\frac{2}{3},\frac{1}{12}$ $0,\frac{1}{2},\frac{1}{12}$

Symmetry operations

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

(1) 1	(2) $3^{+}\ 0,0,z$	(3) $3^{-}\ 0,0,z$
(4) $2\quad x,x,\frac{1}{4}$	(5) $2\quad x,0,\frac{1}{4}$	(6) $2\quad 0,y,\frac{1}{4}$
(7) $\bar{1}\quad 0,0,0$	(8) $\bar{3}^{+}\ 0,0,z;\ \ 0,0,0$	(9) $\bar{3}^{-}\ 0,0,z;\ \ 0,0,0$
(10) $c\quad x,\bar{x},z$	(11) $c\quad x,2x,z$	(12) $c\quad 2x,x,z$

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

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^{+}(0,0,\frac{1}{3})\quad \frac{1}{3},\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{1}{3})\quad \frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{6},\frac{5}{12}$	(5) $2(\frac{1}{2},0,0)\quad x,\frac{1}{6},\frac{5}{12}$	(6) $2\quad \frac{1}{3},y,\frac{5}{12}$
(7) $\bar{1}\quad \frac{1}{3},\frac{1}{6},\frac{1}{6}$	(8) $\bar{3}^{+}\ \frac{1}{3},-\frac{1}{3},z;\ \ \frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(9) $\bar{3}^{-}\ \frac{1}{3},\frac{2}{3},z;\ \ \frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})\quad x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})\quad x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})\quad 2x,x,z$

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

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^{+}(0,0,\frac{2}{3})\quad 0,\frac{1}{3},z$	(3) $3^{-}(0,0,\frac{2}{3})\quad \frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{6},\frac{1}{12}$	(5) $2\quad x,\frac{1}{3},\frac{1}{12}$	(6) $2(0,\frac{1}{2},0)\quad \frac{1}{6},y,\frac{1}{12}$
(7) $\bar{1}\quad \frac{1}{6},\frac{1}{3},\frac{1}{3}$	(8) $\bar{3}^{+}\ \frac{2}{3},\frac{1}{3},z;\ \ \frac{2}{3},\frac{1}{3},\frac{1}{3}$	(9) $\bar{3}^{-}\ -\frac{1}{3},\frac{1}{3},z;\ \ -\frac{1}{3},\frac{1}{3},\frac{1}{3}$
(10) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})\quad x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})\quad 2x-\frac{1}{2},x,z$

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); (7)

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:
36	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) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$				$hki0$: $-h+k=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				$hh\overline{2h}l$: $l=3n$
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$				$h\bar{h}0l$: $h+l=3n,\ l=2n$
									$000l$: $l=6n$
									$h\bar{h}00$: $h=3n$
									Special: as above, plus
18	e	$.2$	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
18	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
12	c	$3.$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
6	b	$\bar{3}.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
6	a	32	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I [2] $R3c$ (161) (1; 2; 3; 10; 11; 12)+
[2] $R32$ (155) (1; 2; 3; 4; 5; 6)+
[2] $R\bar{3}1$ ($R\bar{3}$, 148) (1; 2; 3; 7; 8; 9)+
{ [3] $R12/c$ ($C2/c$, 15) (1; 4; 7; 10)+
{ [3] $R12/c$ ($C2/c$, 15) (1; 5; 7; 11)+
{ [3] $R12/c$ ($C2/c$, 15) (1; 6; 7; 12)+

IIa { [3] $P\bar{3}c1$ (165) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{ [3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
{ [3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 5\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (163)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I [2] $R3c$ (161) 1; 2; 3; 10; 11; 12
[2] $R32$ (155) 1; 2; 3; 4; 5; 6
[2] $R\bar{3}1$ ($R\bar{3}$, 148) 1; 2; 3; 7; 8; 9
{ [3] $R12/c$ ($C2/c$, 15) 1; 4; 7; 10
{ [3] $R12/c$ ($C2/c$, 15) 1; 5; 7; 11
{ [3] $R12/c$ ($C2/c$, 15) 1; 6; 7; 12

IIa none

IIb [3] $P\bar{3}c1$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (165)

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}-\mathbf{c}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}' = \mathbf{a}+2\mathbf{b}+2\mathbf{c}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}+2\mathbf{c}, \mathbf{c}' = 2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \mathbf{b}' = \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}), \mathbf{c}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (166);
[3] $P\bar{3}1c$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (163)

Trigonal	$\bar{3}m$	D_{3d}^{6}	$R\bar{3}c$
Patterson symmetry $R\bar{3}m$		$R\bar{3}2/c$	No. 167

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

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

Asymmetric unit $\frac{1}{4} \le x \le \frac{5}{4}$; $\frac{1}{4} \le y \le \frac{5}{4}$; $\frac{1}{4} \le z \le \frac{3}{4}$; $y \le x$; $z \le \min(y, \frac{3}{2} - x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{5}{4},\frac{1}{4},\frac{1}{4}$ $\frac{5}{4},\frac{5}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$	(5) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(6) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(7) $\bar{1}$ 0,0,0	(8) $\bar{3}^+$ x,x,x; 0,0,0	(9) $\bar{3}^-$ x,x,x; 0,0,0
(10) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(11) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(12) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
12 f 1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl : $l=2n$
	(4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(5) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	hhh : $h=2n$
	(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$	
	(10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	
				Special: as above, plus
6 e .2	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},x,\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{4},x$	$\bar{x},x+\frac{1}{2},\frac{3}{4}$ $\frac{3}{4},\bar{x},x+\frac{1}{2}$ $x+\frac{1}{2},\frac{3}{4},\bar{x}$		no extra conditions
6 d $\bar{1}$	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$		hkl : $h+k+l=2n$
4 c 3.	x,x,x $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$		hkl : $h+k+l=2n$
2 b $\bar{3}$.	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k+l=2n$
2 a 32	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl : $h+k+l=2n$

Symmetry of special projections

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

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

Along $[2\bar{1}\bar{1}]$ $p2gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

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