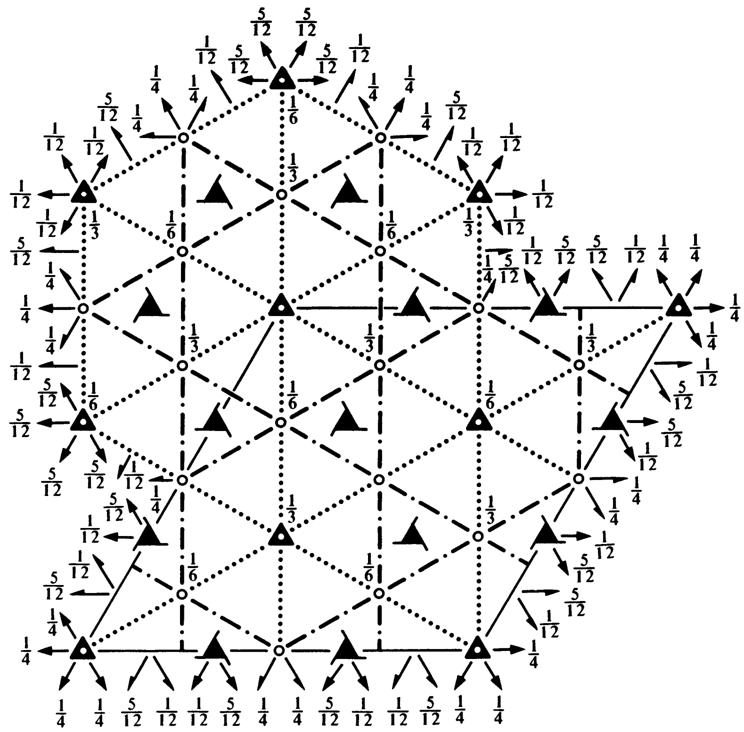
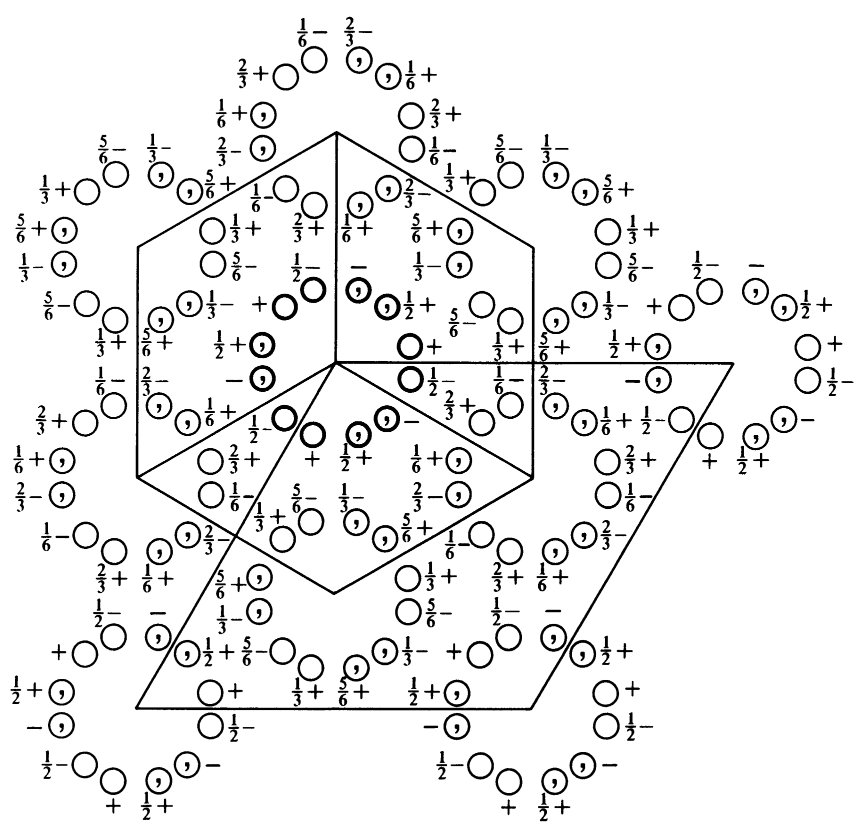
International Tables for Crystallography (2006). Vol. A, Space group 167, pp. 548–551.

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

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

HEXAGONAL AXES





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

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

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

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

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Symmetry operations

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

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

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) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{6},\frac{5}{12}$	(5) $2(\frac{1}{2},0,0)$ $x,\frac{1}{6},\frac{5}{12}$	(6) 2 $\frac{1}{3},y,\frac{5}{12}$
(7) $\bar{1}$ $\frac{1}{3},\frac{1}{6},\frac{1}{6}$	(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) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})$ $x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})$ $2x,x,z$

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) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{6},\frac{1}{12}$	(5) 2 $x,\frac{1}{3},\frac{1}{12}$	(6) $2(0,\frac{1}{2},0)$ $\frac{1}{6},y,\frac{1}{12}$
(7) $\bar{1}$ $\frac{1}{6},\frac{1}{3},\frac{1}{3}$	(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) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})$ $x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ $2x-\frac{1}{2},x,z$

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
(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) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$
(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) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$

hhl : $l=2n$
hhh : $h=2n$

Special: as above, plus

6	e	$.2$	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$; $\bar{x},x+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},x,\bar{x}+\frac{1}{2}$; $\frac{3}{4},\bar{x},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},x$; $x+\frac{1}{2},\frac{3}{4},\bar{x}$			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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