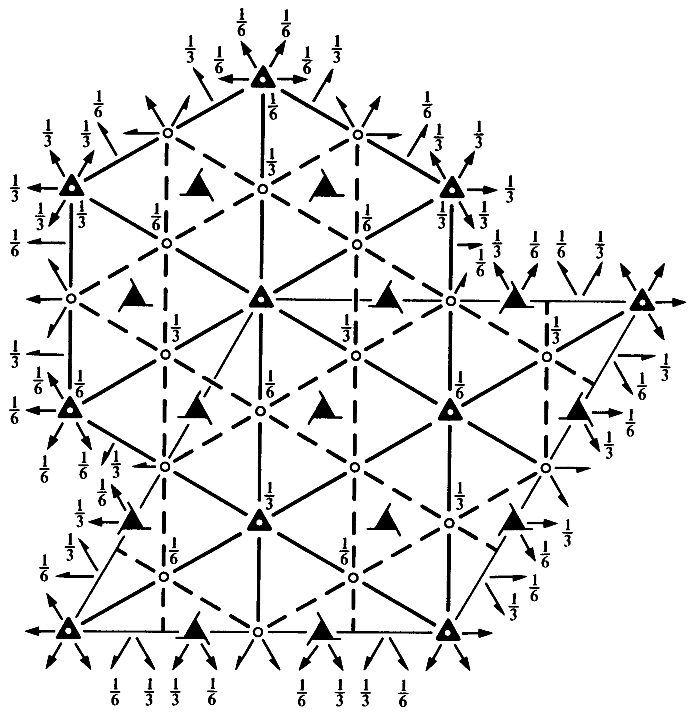
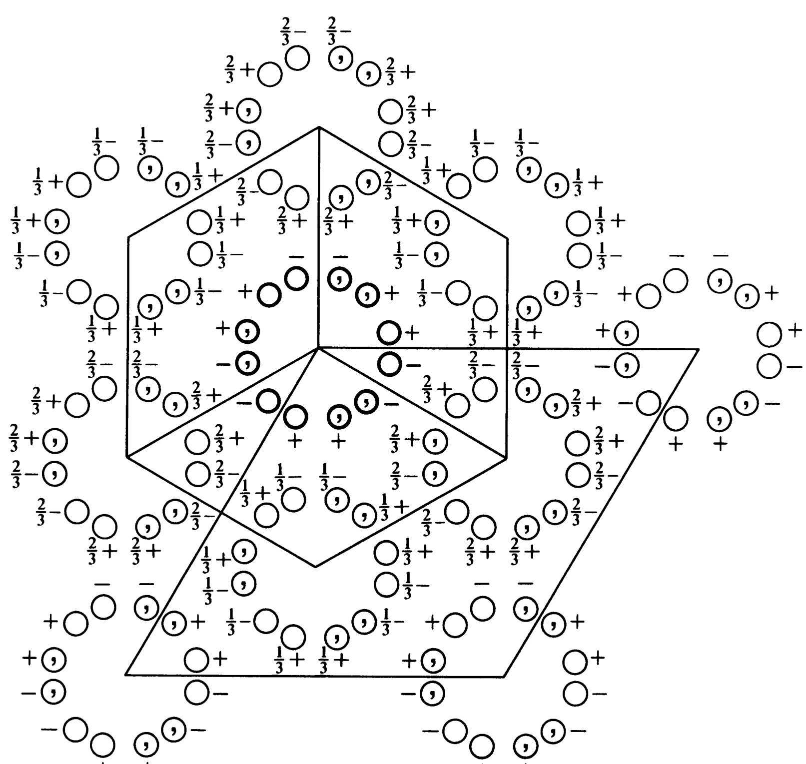
International Tables for Crystallography (2006). Vol. A, Space group 166, pp. 544–547.

$R\bar{3}m$ D_{3d}^{5} $\bar{3}m$ Trigonal

No. 166 $R\bar{3}2/m$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





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

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

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

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

Symmetry operations

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

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

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

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

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); (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	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hkil$: $-h+k+l=3n$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$				$hki0$: $-h+k=3n$
			(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) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$				$h\bar{h}0l$: $h+l=3n$
									$000l$: $l=3n$
									$h\bar{h}00$: $h=3n$
									Special: no extra conditions
18	h	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	
18	g	$.2$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
18	f	$.2$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
9	e	$.2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
9	d	$.2/m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
6	c	$3m$	$0,0,z$	$0,0,\bar{z}$					
3	b	$\bar{3}m$	$0,0,\frac{1}{2}$						
3	a	$\bar{3}m$	$0,0,0$						

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

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I [2] $R3m$ (160) (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] $R12/m$ ($C2/m$, 12) (1; 4; 7; 10)+
{ [3] $R12/m$ ($C2/m$, 12) (1; 5; 7; 11)+
{ [3] $R12/m$ ($C2/m$, 12) (1; 6; 7; 12)+

IIa { [3] $P\bar{3}m1$ (164) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
{ [3] $P\bar{3}m1$ (164) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
{ [3] $P\bar{3}m1$ (164) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$

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

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}, \mathbf{b}' = -\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -2\mathbf{a}, \mathbf{b}' = -2\mathbf{b}$) (166)

Minimal non-isomorphic supergroups

I [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b}), \mathbf{c}' = \frac{1}{3}\mathbf{c}$) (162)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I [2] $R3m$ (160) 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] $R12/m$ ($C2/m$, 12) 1; 4; 7; 10
{ [3] $R12/m$ ($C2/m$, 12) 1; 5; 7; 11
{ [3] $R12/m$ ($C2/m$, 12) 1; 6; 7; 12

IIa none

IIb [2] $F\bar{3}c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($R\bar{3}c$, 167); [3] $P\bar{3}m1$ ($\mathbf{a}' = \mathbf{a}-\mathbf{b}, \mathbf{b}' = \mathbf{b}-\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$) (164)

Maximal isomorphic subgroups of lowest index

IIc [2] $R\bar{3}m$ ($\mathbf{a}' = \mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}$) (166); [4] $R\bar{3}m$ ($\mathbf{a}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}, \mathbf{b}' = \mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{c}' = \mathbf{a}+\mathbf{b}-\mathbf{c}$) (166)

Minimal non-isomorphic supergroups

I [4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II [3] $P\bar{3}1m$ ($\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}), \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}), \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (162)

Trigonal $\bar{3}m$ D_{3d}^5 $R\bar{3}m$

Patterson symmetry $R\bar{3}m$ $R\bar{3}2/m$ No. 166

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

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

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

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

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x},0,x$	(5) 2 $x,\bar{x},0$	(6) 2 $0,y,\bar{y}$
(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) m x,y,x	(11) m x,x,z	(12) m 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	i	1	(1) x,y,z	(2) z,x,y	(3) y,z,x				no conditions
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$				
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$				
			(10) z,y,x	(11) y,x,z	(12) x,z,y				
									Special: no extra conditions
6	h	$.m$	x,x,z	z,x,x	x,z,x	$\bar{z},\bar{x},\bar{x}$	$\bar{x},\bar{x},\bar{z}$	$\bar{x},\bar{z},\bar{x}$	
6	g	$.2$	$x,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\bar{x}$	$\bar{x},\frac{1}{2},x$	$\bar{x},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},x$	$x,\frac{1}{2},\bar{x}$	
6	f	$.2$	$x,\bar{x},0$	$0,x,\bar{x}$	$\bar{x},0,x$	$\bar{x},x,0$	$0,\bar{x},x$	$x,0,\bar{x}$	
3	e	$.2/m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
3	d	$.2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
2	c	$3m$	x,x,x	$\bar{x},\bar{x},\bar{x}$					
1	b	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	$\bar{3}m$	$0,0,0$						

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

Along $[2\bar{1}\bar{1}]$ $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

(*Continued on preceding page*)