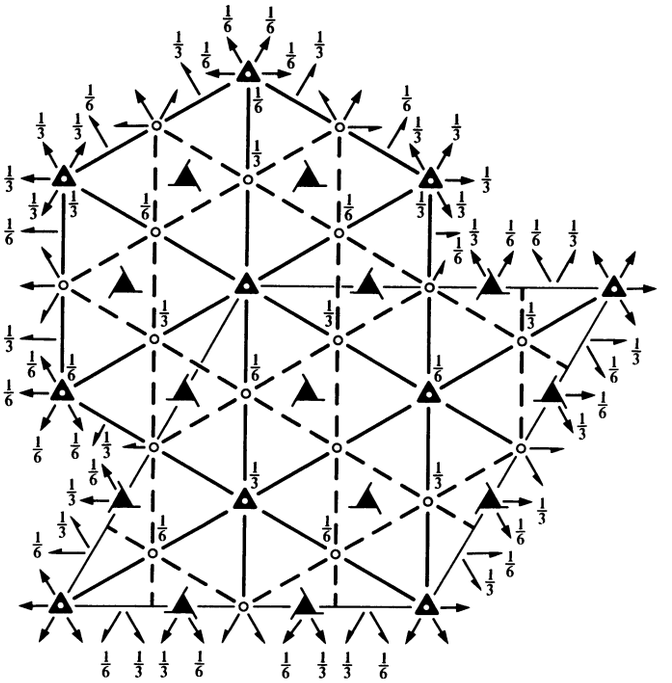
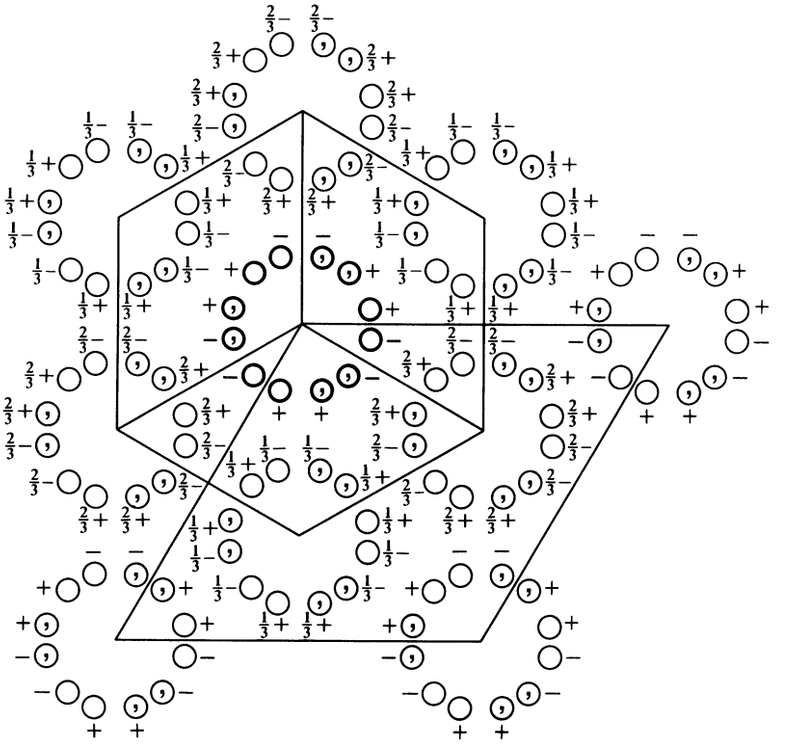
$R\bar{3}m$ D_{3d}^5 $\bar{3}m$ Trigonal

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
36	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	General:
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	$hkil$: $-h+k+l=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	$hki0$: $-h+k=3n$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$	$h\bar{h}2\bar{h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$
						$000l$: $l=3n$
						$h\bar{h}00$: $h=3n$
						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	3 m	$0,0,z$	$0,0,\bar{z}$		
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 $0,0,z$

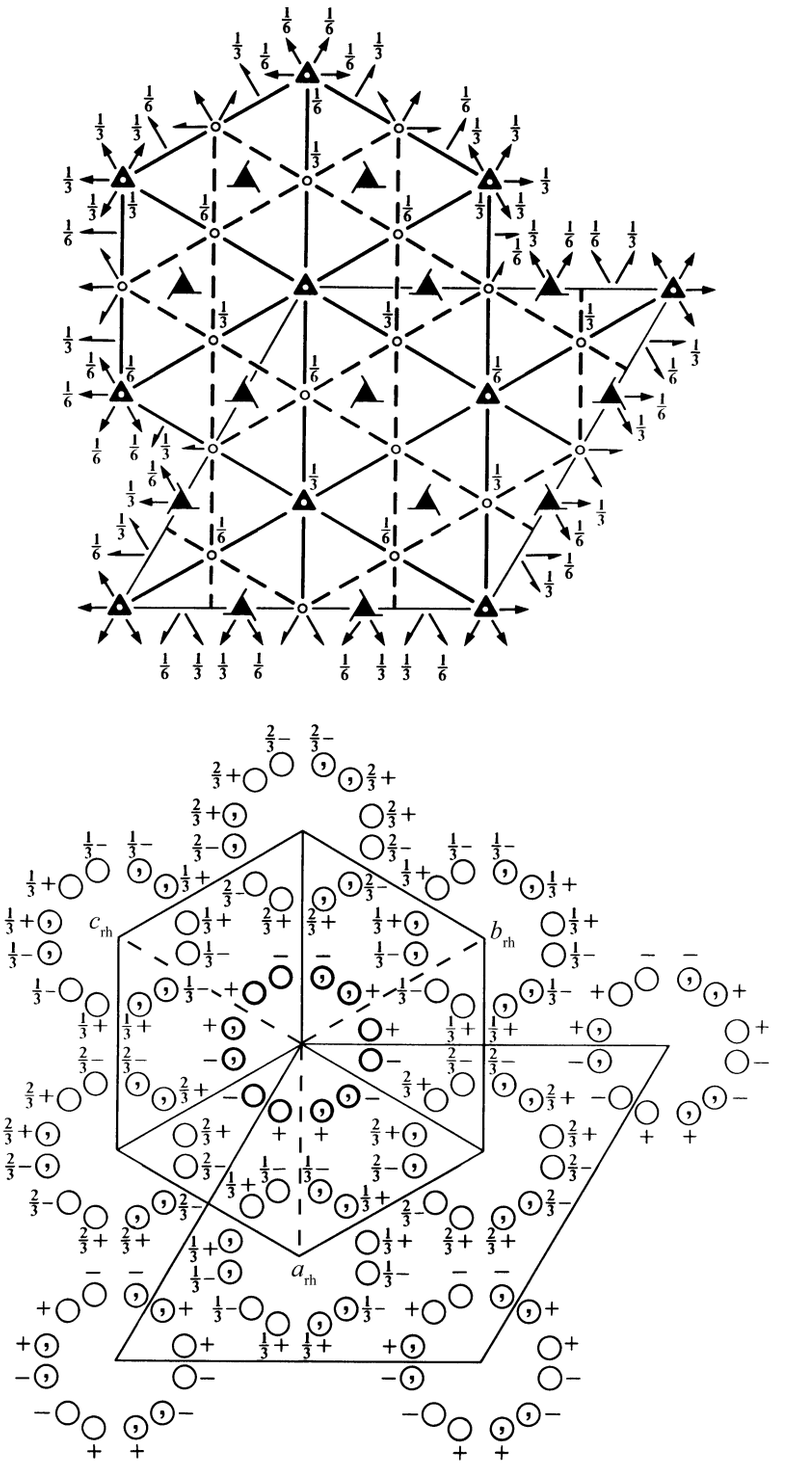
Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

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

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

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

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

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

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

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,y,x	x,x,y	y,x,x	$\bar{x},\bar{y},\bar{x}$ $\bar{y},\bar{x},\bar{x}$ $\bar{x},\bar{x},\bar{y}$
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	$.2/m$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	
3	d	$.2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	
2	c	$3\,m$	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 $2x,\bar{x},\bar{x}$