

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates						Reflection conditions
								$h, k, l$ permutable
								General:
48	$n$ 1	(1) $x, y, z$ (5) $z, x, y$ (9) $y, z, x$ (13) $y, x, \bar{z}$ (17) $x, z, \bar{y}$ (21) $z, y, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y}, \bar{x}, z$ (41) $\bar{x}, \bar{z}, y$ (45) $\bar{z}, \bar{y}, x$	(2) $\bar{x}, \bar{y}, z$ (6) $z, \bar{x}, \bar{y}$ (10) $\bar{y}, z, \bar{x}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (18) $\bar{x}, z, y$ (22) $z, \bar{y}, x$ (26) $x, y, \bar{z}$ (30) $\bar{z}, x, y$ (34) $y, \bar{z}, x$ (38) $y, x, z$ (42) $x, \bar{z}, \bar{y}$ (46) $\bar{z}, y, \bar{x}$	(3) $\bar{x}, y, \bar{z}$ (7) $\bar{z}, \bar{x}, y$ (11) $y, \bar{z}, \bar{x}$ (15) $y, \bar{x}, z$ (19) $\bar{x}, \bar{z}, \bar{y}$ (23) $\bar{z}, y, x$ (27) $x, \bar{y}, z$ (31) $z, x, \bar{y}$ (35) $\bar{y}, z, x$ (39) $\bar{y}, x, \bar{z}$ (43) $x, z, y$ (47) $z, \bar{y}, \bar{x}$	(4) $x, \bar{y}, \bar{z}$ (8) $\bar{z}, x, \bar{y}$ (12) $\bar{y}, \bar{z}, x$ (16) $\bar{y}, x, z$ (20) $x, \bar{z}, y$ (24) $\bar{z}, \bar{y}, \bar{x}$ (28) $\bar{x}, y, z$ (32) $z, \bar{x}, y$ (36) $y, z, \bar{x}$ (40) $y, \bar{x}, \bar{z}$ (44) $\bar{x}, z, \bar{y}$ (48) $z, y, x$			no conditions
24	$m$ . . $m$	$x, x, z$ $\bar{z}, \bar{x}, x$ $x, x, \bar{z}$ $\bar{x}, \bar{z}, \bar{x}$	$\bar{x}, \bar{x}, z$ $\bar{z}, x, \bar{x}$ $\bar{x}, \bar{x}, \bar{z}$ $x, \bar{z}, x$	$\bar{x}, x, \bar{z}$ $x, z, x$ $x, \bar{x}, z$ $z, x, \bar{x}$	$x, \bar{x}, \bar{z}$ $\bar{x}, z, \bar{x}$ $\bar{x}, x, z$ $z, \bar{x}, x$	$z, x, x$ $x, \bar{z}, \bar{x}$ $x, z, \bar{x}$ $\bar{z}, x, x$	$z, \bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$ $\bar{x}, z, x$ $\bar{z}, \bar{x}, \bar{x}$	Special: no extra conditions
24	$l$ $m$ . .	$\frac{1}{2}, y, z$ $\bar{z}, \frac{1}{2}, y$ $y, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \bar{z}, \bar{y}$	$\frac{1}{2}, \bar{y}, z$ $\bar{z}, \frac{1}{2}, \bar{y}$ $\bar{y}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \bar{z}, y$	$\frac{1}{2}, y, \bar{z}$ $y, z, \frac{1}{2}$ $y, \frac{1}{2}, z$ $z, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{z}$ $\bar{y}, z, \frac{1}{2}$ $\bar{y}, \frac{1}{2}, z$ $z, \bar{y}, \frac{1}{2}$	$z, \frac{1}{2}, y$ $y, \bar{z}, \frac{1}{2}$ $\frac{1}{2}, z, \bar{y}$ $\bar{z}, y, \frac{1}{2}$	$z, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{z}, \frac{1}{2}$ $\frac{1}{2}, z, y$ $\bar{z}, \bar{y}, \frac{1}{2}$	
24	$k$ $m$ . .	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	
12	$j$ $m$ . $m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	
12	$i$ $m$ . $m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	
12	$h$ $m$ $m2$ . .	$x, \frac{1}{2}, 0$ $\frac{1}{2}, x, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x}, 0$	$0, x, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, x$ $0, \frac{1}{2}, \bar{x}$	$\frac{1}{2}, 0, \bar{x}$ $0, \frac{1}{2}, x$	
8	$g$ . $3m$	$x, x, x$ $x, x, \bar{x}$	$\bar{x}, \bar{x}, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x}, x, \bar{x}$ $x, \bar{x}, x$	$x, \bar{x}, \bar{x}$ $\bar{x}, x, x$			
6	$f$ $4m$ . $m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$	
6	$e$ $4m$ . $m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	
3	$d$ $4/m$ $m$ . $m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$				
3	$c$ $4/m$ $m$ . $m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$				
1	$b$ $m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						
1	$a$ $m\bar{3}m$	$0, 0, 0$						

**Symmetry of special projections**

Along  $[001]$   $p4mm$   
 $\mathbf{a}' = \mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

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  $[110]$   $p2mm$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, x, 0$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ ; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Reflection conditions
96 <i>l</i> 1	(1) $x, y, z$ (2) $\bar{x}, \bar{y}, z$ (3) $\bar{x}, y, \bar{z}$ (4) $x, \bar{y}, \bar{z}$ (5) $z, x, y$ (6) $z, \bar{x}, \bar{y}$ (7) $\bar{z}, \bar{x}, y$ (8) $\bar{z}, x, \bar{y}$ (9) $y, z, x$ (10) $\bar{y}, z, \bar{x}$ (11) $y, \bar{z}, \bar{x}$ (12) $\bar{y}, \bar{z}, x$ (13) $y, x, \bar{z}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (15) $y, \bar{x}, z$ (16) $\bar{y}, x, z$ (17) $x, z, \bar{y}$ (18) $\bar{x}, z, y$ (19) $\bar{x}, \bar{z}, \bar{y}$ (20) $x, \bar{z}, y$ (21) $z, y, \bar{x}$ (22) $z, \bar{y}, x$ (23) $\bar{z}, y, x$ (24) $\bar{z}, \bar{y}, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (26) $x, y, \bar{z}$ (27) $x, \bar{y}, z$ (28) $\bar{x}, y, z$ (29) $\bar{z}, \bar{x}, \bar{y}$ (30) $\bar{z}, x, y$ (31) $z, x, \bar{y}$ (32) $z, \bar{x}, y$ (33) $\bar{y}, \bar{z}, \bar{x}$ (34) $y, \bar{z}, x$ (35) $\bar{y}, z, x$ (36) $y, z, \bar{x}$ (37) $\bar{y}, \bar{x}, z$ (38) $y, x, z$ (39) $\bar{y}, x, \bar{z}$ (40) $y, \bar{x}, \bar{z}$ (41) $\bar{x}, \bar{z}, y$ (42) $x, \bar{z}, \bar{y}$ (43) $x, z, y$ (44) $\bar{x}, z, \bar{y}$ (45) $\bar{z}, \bar{y}, x$ (46) $\bar{z}, y, \bar{x}$ (47) $z, \bar{y}, \bar{x}$ (48) $z, y, x$	<p><math>hkl : h + k + l = 2n</math>  <math>0kl : k + l = 2n</math>  <math>hhl : l = 2n</math>  <math>h00 : h = 2n</math></p>
48 <i>k</i> $\dots m$	$x, x, z$ $\bar{x}, \bar{x}, z$ $\bar{x}, x, \bar{z}$ $x, \bar{x}, \bar{z}$ $z, x, x$ $z, \bar{x}, \bar{x}$ $\bar{z}, \bar{x}, x$ $\bar{z}, x, \bar{x}$ $x, z, x$ $\bar{x}, z, \bar{x}$ $x, \bar{z}, \bar{x}$ $\bar{x}, \bar{z}, x$ $x, x, \bar{z}$ $\bar{x}, \bar{x}, \bar{z}$ $x, \bar{x}, z$ $\bar{x}, x, z$ $x, z, \bar{x}$ $\bar{x}, z, x$ $\bar{x}, \bar{z}, \bar{x}$ $x, \bar{z}, x$ $z, x, \bar{x}$ $z, \bar{x}, x$ $\bar{z}, x, x$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
48 <i>j</i> $m \dots$	$0, y, z$ $0, \bar{y}, z$ $0, y, \bar{z}$ $0, \bar{y}, \bar{z}$ $z, 0, y$ $z, 0, \bar{y}$ $\bar{z}, 0, y$ $\bar{z}, 0, \bar{y}$ $y, z, 0$ $\bar{y}, z, 0$ $y, \bar{z}, 0$ $\bar{y}, \bar{z}, 0$ $y, 0, \bar{z}$ $\bar{y}, 0, \bar{z}$ $y, 0, z$ $\bar{y}, 0, z$ $0, z, \bar{y}$ $0, z, y$ $0, \bar{z}, \bar{y}$ $0, \bar{z}, y$ $z, y, 0$ $z, \bar{y}, 0$ $\bar{z}, y, 0$ $\bar{z}, \bar{y}, 0$	no extra conditions
48 <i>i</i> $\dots 2$	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\frac{3}{4}, y, y + \frac{1}{2}$ $\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $\frac{1}{4}, y, y + \frac{1}{2}$ $\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $y + \frac{1}{2}, \frac{1}{4}, y$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $y, y + \frac{1}{2}, \frac{1}{4}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$	no extra conditions
24 <i>h</i> $m \dots m2$	$0, y, y$ $0, \bar{y}, y$ $0, y, \bar{y}$ $0, \bar{y}, \bar{y}$ $y, 0, y$ $y, 0, \bar{y}$ $\bar{y}, 0, y$ $\bar{y}, 0, \bar{y}$ $y, y, 0$ $\bar{y}, y, 0$ $y, \bar{y}, 0$ $\bar{y}, \bar{y}, 0$	no extra conditions
24 <i>g</i> $m m 2 \dots$	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, x, 0$ $\frac{1}{2}, \bar{x}, 0$ $0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x}$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$ $x, \frac{1}{2}, 0$ $\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \bar{x}$ $\frac{1}{2}, 0, x$	no extra conditions
16 <i>f</i> $\dots 3m$	$x, x, x$ $\bar{x}, \bar{x}, x$ $\bar{x}, x, \bar{x}$ $x, \bar{x}, \bar{x}$ $x, x, \bar{x}$ $\bar{x}, \bar{x}, \bar{x}$ $x, \bar{x}, x$ $\bar{x}, x, x$	no extra conditions
12 <i>e</i> $4m \dots m$	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $0, 0, x$ $0, 0, \bar{x}$	no extra conditions
12 <i>d</i> $\bar{4}m \dots 2$	$\frac{1}{4}, 0, \frac{1}{2}$ $\frac{3}{4}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{4}, 0$ $\frac{1}{2}, \frac{3}{4}, 0$ $0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	no extra conditions
8 <i>c</i> $\dots \bar{3}m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : k, l = 2n$
6 <i>b</i> $4/m m \dots m$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions
2 <i>a</i> $m \bar{3}m$	$0, 0, 0$	no extra conditions

**Symmetry of special projections**

Along [001]  $p4mm$

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$   $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$

Origin at 0,0,z

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 [110]  $p2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$   $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at x,x,0

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ;  $t(\frac{1}{2}, 0, \frac{1}{2})$ ; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates							Reflection conditions
	$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$				$h, k, l$ permutable General:
192 $l$ 1	(1) $x, y, z$ (5) $z, x, y$ (9) $y, z, x$ (13) $y, x, \bar{z}$ (17) $x, z, \bar{y}$ (21) $z, y, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y}, \bar{x}, z$ (41) $\bar{x}, \bar{z}, y$ (45) $\bar{z}, \bar{y}, x$	(2) $\bar{x}, \bar{y}, z$ (6) $z, \bar{x}, \bar{y}$ (10) $\bar{y}, z, \bar{x}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (18) $\bar{x}, z, y$ (22) $z, \bar{y}, x$ (26) $x, y, \bar{z}$ (30) $\bar{z}, x, y$ (34) $y, \bar{z}, x$ (38) $y, x, z$ (42) $x, \bar{z}, \bar{y}$ (46) $\bar{z}, y, \bar{x}$	(3) $\bar{x}, y, \bar{z}$ (7) $\bar{z}, \bar{x}, y$ (11) $y, \bar{z}, \bar{x}$ (15) $y, \bar{x}, z$ (19) $\bar{x}, \bar{z}, \bar{y}$ (23) $\bar{z}, y, x$ (27) $x, \bar{y}, z$ (31) $z, x, \bar{y}$ (35) $\bar{y}, z, x$ (39) $\bar{y}, x, \bar{z}$ (43) $x, z, y$ (47) $z, \bar{y}, \bar{x}$	(4) $x, \bar{y}, \bar{z}$ (8) $\bar{z}, x, \bar{y}$ (12) $\bar{y}, \bar{z}, x$ (16) $\bar{y}, x, z$ (20) $x, \bar{z}, y$ (24) $\bar{z}, \bar{y}, \bar{x}$ (28) $\bar{x}, y, z$ (32) $z, \bar{x}, y$ (36) $y, z, \bar{x}$ (40) $y, \bar{x}, \bar{z}$ (44) $\bar{x}, z, \bar{y}$ (48) $z, y, x$	$hkl : h+k, h+l, k+l = 2n$ $OkI : k, l = 2n$ $hhl : h+l = 2n$ $h00 : h = 2n$			
96 $k$ $\dots m$	$x, x, z$ $\bar{z}, \bar{x}, x$ $x, x, \bar{z}$ $\bar{x}, \bar{z}, \bar{x}$	$\bar{x}, \bar{x}, z$ $\bar{z}, x, \bar{x}$ $\bar{x}, \bar{x}, \bar{z}$ $x, \bar{z}, x$	$\bar{x}, x, \bar{z}$ $x, z, x$ $x, \bar{x}, z$ $z, x, \bar{x}$	$x, \bar{x}, \bar{z}$ $\bar{x}, z, \bar{x}$ $\bar{x}, x, z$ $z, \bar{x}, x$	$z, x, x$ $x, \bar{z}, \bar{x}$ $x, z, \bar{x}$ $\bar{z}, x, x$	$z, \bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$ $\bar{x}, z, x$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions	
96 $j$ $m \dots$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions	
48 $i$ $m \dots m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	no extra conditions	
48 $h$ $m \dots m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions	
48 $g$ $2 \dots mm$	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$	$hkl : h = 2n$	
32 $f$ $\dots 3m$	$x, x, x$ $x, x, \bar{x}$	$\bar{x}, \bar{x}, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x}, x, \bar{x}$ $x, \bar{x}, x$	$x, \bar{x}, \bar{x}$ $\bar{x}, x, x$			no extra conditions	
24 $e$ $4m \dots m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions	
24 $d$ $m \dots mm$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h = 2n$	
8 $c$ $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$					$hkl : h = 2n$	
4 $b$ $m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions	
4 $a$ $m\bar{3}m$	$0, 0, 0$						no extra conditions	

**Symmetry of special projections**

Along  $[001]$   $p4mm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$      $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[111]$   $p6mm$   
 $\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$      $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$   
 Origin at  $x, x, x$

Along  $[110]$   $c2mm$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, x, 0$

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ;  $t(\frac{1}{2}, 0, \frac{1}{2})$ ; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions					
	$(0,0,0)+$ $(0, \frac{1}{2}, \frac{1}{2})+$ $(\frac{1}{2}, 0, \frac{1}{2})+$ $(\frac{1}{2}, \frac{1}{2}, 0)+$	$h, k, l$ permutable General:					
192 <i>i</i> 1	(1) $x, y, z$ (5) $z, x, y$ (9) $y, z, x$ (13) $y + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (17) $x + \frac{3}{4}, z + \frac{1}{4}, \bar{y} + \frac{3}{4}$ (21) $z + \frac{3}{4}, y + \frac{1}{4}, \bar{x} + \frac{3}{4}$ (25) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (29) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (33) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ (37) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(2) $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $z + \frac{1}{2}, \bar{x}, \bar{y} + \frac{1}{2}$ (10) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ (14) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (18) $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, y + \frac{1}{4}$ (22) $z + \frac{1}{4}, \bar{y} + \frac{3}{4}, x + \frac{3}{4}$ (26) $x + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (30) $\bar{z} + \frac{3}{4}, x + \frac{1}{4}, y + \frac{3}{4}$ (34) $y + \frac{3}{4}, \bar{z} + \frac{3}{4}, x + \frac{1}{4}$ (38) $y, x, z$ (42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y}$ (46) $\bar{z}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) $\bar{z}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (11) $y + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$ (15) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ (19) $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$ (23) $\bar{z} + \frac{3}{4}, y + \frac{3}{4}, x + \frac{1}{4}$ (27) $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, z + \frac{1}{4}$ (31) $z + \frac{1}{4}, x + \frac{3}{4}, \bar{y} + \frac{3}{4}$ (35) $\bar{y} + \frac{3}{4}, z + \frac{1}{4}, x + \frac{3}{4}$ (39) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (43) $x, z, y$ (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x}$	(4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (12) $\bar{y}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ (16) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (20) $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, y + \frac{3}{4}$ (24) $\bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ (28) $\bar{x} + \frac{3}{4}, y + \frac{1}{4}, z + \frac{3}{4}$ (32) $z + \frac{3}{4}, \bar{x} + \frac{3}{4}, y + \frac{1}{4}$ (36) $y + \frac{1}{4}, z + \frac{3}{4}, \bar{x} + \frac{3}{4}$ (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (44) $\bar{x}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (48) $z, y, x$	$hkl : h + k = 2n$ and $h + l, k + l = 2n$ $OkI : k + l = 4n$ and $k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 4n$		
96 <i>h</i> .. 2	$\frac{1}{8}, y, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \frac{1}{8}, y$ $y, \bar{y} + \frac{1}{4}, \frac{1}{8}$ $\frac{1}{8}, \bar{y} + \frac{1}{4}, y$ $y, \frac{1}{8}, \bar{y} + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, y, \frac{1}{8}$	$\frac{7}{8}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \frac{7}{8}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{3}{4}, \frac{7}{8}$ $\frac{3}{8}, y + \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{8}, y + \frac{3}{4}$ $y + \frac{3}{4}, y + \frac{1}{2}, \frac{3}{8}$	$\frac{3}{8}, y + \frac{1}{2}, y + \frac{3}{4}$ $y + \frac{3}{4}, \frac{3}{8}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{8}$ $\frac{7}{8}, \bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{7}{8}, \bar{y} + \frac{3}{4}$ $\bar{y} + \frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{7}{8}$	$\frac{5}{8}, \bar{y}, y + \frac{1}{4}$ $y + \frac{1}{4}, \frac{5}{8}, \bar{y}$ $\bar{y}, y + \frac{1}{4}, \frac{5}{8}$ $\frac{5}{8}, y + \frac{1}{4}, \bar{y}$ $\bar{y}, \frac{5}{8}, y + \frac{1}{4}$ $y + \frac{1}{4}, \bar{y}, \frac{5}{8}$	no extra conditions		
96 <i>g</i> .. <i>m</i>	$x, x, z$ $z, x, x$ $x, z, x$ $x + \frac{3}{4}, x + \frac{1}{4}, \bar{z} + \frac{3}{4}$ $x + \frac{3}{4}, z + \frac{1}{4}, \bar{x} + \frac{3}{4}$ $z + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ $\bar{x} + \frac{3}{4}, z + \frac{3}{4}, x + \frac{1}{4}$ $z + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $\bar{z}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$ $\bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ $\bar{z} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$	$x + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $\bar{x}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ $x + \frac{1}{4}, \bar{z} + \frac{3}{4}, x + \frac{3}{4}$ $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	no extra conditions		
48 <i>f</i> 2. <i>mm</i>	$x, 0, 0$ $\frac{3}{4}, x + \frac{1}{4}, \frac{3}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{4}, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$0, x, 0$ $x + \frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$0, 0, x$ $\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{3}{4}$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x + \frac{3}{4}$	$hkl : h = 2n + 1$ or $h + k + l = 4n$
32 <i>e</i> . 3 <i>m</i>	$x, x, x$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $x + \frac{3}{4}, x + \frac{1}{4}, \bar{x} + \frac{3}{4}$ $x + \frac{1}{4}, \bar{x} + \frac{3}{4}, x + \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{x} + \frac{1}{4}$ $\bar{x} + \frac{3}{4}, x + \frac{3}{4}, x + \frac{1}{4}$				no extra conditions	
16 <i>d</i> . $\bar{3}m$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{3}{8}, \frac{7}{8}, \frac{1}{8}$ $\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{3}{8}$ $\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{3}{8}, \frac{7}{8}$ $\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$		$hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$	
16 <i>c</i> . $\bar{3}m$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{7}{8}$	$\frac{5}{8}, \frac{7}{8}, \frac{3}{8}$		$hkl : h = 2n + 1$ or $h + k + l = 4n$	
8 <i>b</i> $\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$				$hkl : h = 2n + 1$ or $h + k + l = 4n$	
8 <i>a</i> $\bar{4}3m$	$0, 0, 0$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$					

**Symmetry of special projections**

Along [001]  $p4mm$

$\mathbf{a}' = \frac{1}{4}(\mathbf{a} - \mathbf{b})$      $\mathbf{b}' = \frac{1}{4}(\mathbf{a} + \mathbf{b})$

Origin at 0, 0, z

Along [111]  $p6mm$

$\mathbf{a}' = \frac{1}{6}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$      $\mathbf{b}' = \frac{1}{6}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$

Origin at x, x, x

Along [110]  $c2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$      $\mathbf{b}' = \mathbf{c}$

Origin at x, x,  $\frac{1}{8}$

## Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3 <sup>+</sup> x,x,x	(6) 3 <sup>+</sup> $\bar{x}$ ,x, $\bar{x}$	(7) 3 <sup>+</sup> x, $\bar{x}$ , $\bar{x}$	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}$ ,x
(9) 3 <sup>-</sup> x,x,x	(10) 3 <sup>-</sup> x, $\bar{x}$ , $\bar{x}$	(11) 3 <sup>-</sup> $\bar{x}$ , $\bar{x}$ ,x	(12) 3 <sup>-</sup> $\bar{x}$ ,x, $\bar{x}$
(13) m x,x,z	(14) m x, $\bar{x}$ ,z	(15) $\bar{4}^+$ 0,0,z; 0,0,0	(16) $\bar{4}^-$ 0,0,z; 0,0,0
(17) m x,y,y	(18) $\bar{4}^+$ x,0,0; 0,0,0	(19) $\bar{4}^-$ x,0,0; 0,0,0	(20) m x,y, $\bar{y}$
(21) m x,y,x	(22) $\bar{4}^-$ 0,y,0; 0,0,0	(23) m $\bar{x}$ ,y,x	(24) $\bar{4}^+$ 0,y,0; 0,0,0

For (0, $\frac{1}{2}$ , $\frac{1}{2}$ )+ set

(1) $t(0, \frac{1}{2}, \frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$ ) 0, $\frac{1}{4}$ ,z	(3) 2(0, $\frac{1}{2}$ ,0) 0,y, $\frac{1}{4}$	(4) 2 x, $\frac{1}{4}$ , $\frac{1}{4}$
(5) 3 <sup>+</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $-\frac{1}{3}$ ,x $-\frac{1}{6}$ ,x	(6) 3 <sup>+</sup> $\bar{x}$ ,x $+\frac{1}{2}$ , $\bar{x}$	(7) 3 <sup>+</sup> ( $-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $+\frac{1}{3}$ , $\bar{x}-\frac{1}{6}$ , $\bar{x}$	(8) 3 <sup>+</sup> $\bar{x}$ , $\bar{x}+\frac{1}{2}$ ,x
(9) 3 <sup>-</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $-\frac{1}{6}$ ,x $+\frac{1}{6}$ ,x	(10) 3 <sup>-</sup> ( $-\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $+\frac{1}{6}$ , $\bar{x}+\frac{1}{6}$ , $\bar{x}$	(11) 3 <sup>-</sup> $\bar{x}+\frac{1}{2}$ , $\bar{x}+\frac{1}{2}$ ,x	(12) 3 <sup>-</sup> $\bar{x}-\frac{1}{2}$ ,x $+\frac{1}{2}$ , $\bar{x}$
(13) g( $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ ) x $-\frac{1}{4}$ ,x,z	(14) g( $-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ ) x $+\frac{1}{4}$ , $\bar{x}$ ,z	(15) $\bar{4}^+$ $\frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(16) $\bar{4}^-$ $-\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
(17) g(0, $\frac{1}{2}, \frac{1}{2}$ ) x,y,y	(18) $\bar{4}^+$ x, $\frac{1}{2}$ ,0; 0, $\frac{1}{2}$ ,0	(19) $\bar{4}^-$ x,0, $\frac{1}{2}$ ; 0,0, $\frac{1}{2}$	(20) m x,y $+\frac{1}{2}$ , $\bar{y}$
(21) g( $\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$ ) x $-\frac{1}{4}$ ,y,x	(22) $\bar{4}^-$ $\frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(23) g( $-\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$ ) $\bar{x}+\frac{1}{4}$ ,y,x	(24) $\bar{4}^+$ $-\frac{1}{4}, y, \frac{1}{4}; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

For ( $\frac{1}{2}$ ,0, $\frac{1}{2}$ )+ set

(1) $t(\frac{1}{2}, 0, \frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$ ) $\frac{1}{4}$ ,0,z	(3) 2 $\frac{1}{4}, y, \frac{1}{4}$	(4) 2( $\frac{1}{2}$ ,0,0) x,0, $\frac{1}{4}$
(5) 3 <sup>+</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $+\frac{1}{6}$ ,x $-\frac{1}{6}$ ,x	(6) 3 <sup>+</sup> ( $\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$ ) $\bar{x}+\frac{1}{6}$ ,x $+\frac{1}{6}$ , $\bar{x}$	(7) 3 <sup>+</sup> x $+\frac{1}{2}$ , $\bar{x}-\frac{1}{2}$ , $\bar{x}$	(8) 3 <sup>+</sup> $\bar{x}+\frac{1}{2}$ , $\bar{x}+\frac{1}{2}$ ,x
(9) 3 <sup>-</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $-\frac{1}{6}$ ,x $-\frac{1}{3}$ ,x	(10) 3 <sup>-</sup> x $+\frac{1}{2}$ , $\bar{x}, \bar{x}$	(11) 3 <sup>-</sup> $\bar{x}+\frac{1}{2}$ , $\bar{x}, x$	(12) 3 <sup>-</sup> ( $\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$ ) $\bar{x}-\frac{1}{6}$ ,x $+\frac{1}{3}$ , $\bar{x}$
(13) g( $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ ) x $+\frac{1}{4}$ ,x,z	(14) g( $\frac{1}{4}, -\frac{1}{4}, \frac{1}{2}$ ) x $+\frac{1}{4}$ , $\bar{x}$ ,z	(15) $\bar{4}^+$ $\frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$	(16) $\bar{4}^-$ $\frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
(17) g( $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ ) x,y $-\frac{1}{4}$ ,y	(18) $\bar{4}^+$ x, $\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(19) $\bar{4}^-$ x, $-\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$	(20) g( $\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}$ ) x,y $+\frac{1}{4}$ , $\bar{y}$
(21) g( $\frac{1}{2}, 0, \frac{1}{2}$ ) x,y,x	(22) $\bar{4}^-$ $\frac{1}{2}, y, 0; \frac{1}{2}, 0, 0$	(23) m $\bar{x}+\frac{1}{2}$ ,y,x	(24) $\bar{4}^+$ 0,y, $\frac{1}{2}$ ; 0,0, $\frac{1}{2}$

For ( $\frac{1}{2}$ , $\frac{1}{2}$ ,0)+ set

(1) $t(\frac{1}{2}, \frac{1}{2}, 0)$	(2) 2 $\frac{1}{4}, \frac{1}{4}, z$	(3) 2(0, $\frac{1}{2}$ ,0) $\frac{1}{4}$ ,y,0	(4) 2( $\frac{1}{2}$ ,0,0) x, $\frac{1}{4}$ ,0
(5) 3 <sup>+</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $+\frac{1}{6}$ ,x $+\frac{1}{3}$ ,x	(6) 3 <sup>+</sup> $\bar{x}+\frac{1}{2}$ ,x, $\bar{x}$	(7) 3 <sup>+</sup> x $+\frac{1}{2}$ , $\bar{x}, \bar{x}$	(8) 3 <sup>+</sup> ( $\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$ ) $\bar{x}+\frac{1}{6}$ , $\bar{x}+\frac{1}{3}$ ,x
(9) 3 <sup>-</sup> ( $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ ) x $+\frac{1}{3}$ ,x $+\frac{1}{6}$ ,x	(10) 3 <sup>-</sup> x, $\bar{x}+\frac{1}{2}$ , $\bar{x}$	(11) 3 <sup>-</sup> ( $\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}$ ) $\bar{x}+\frac{1}{3}$ , $\bar{x}+\frac{1}{6}$ ,x	(12) 3 <sup>-</sup> $\bar{x}, x+\frac{1}{2}$ , $\bar{x}$
(13) g( $\frac{1}{2}, \frac{1}{2}, 0$ ) x,x,z	(14) m x $+\frac{1}{2}$ , $\bar{x}, z$	(15) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$	(16) $\bar{4}^-$ 0, $\frac{1}{2}, z; 0, \frac{1}{2}, 0$
(17) g( $\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ ) x,y $+\frac{1}{4}$ ,y	(18) $\bar{4}^+$ x, $\frac{1}{4}, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$	(19) $\bar{4}^-$ x, $\frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(20) g( $\frac{1}{2}, -\frac{1}{4}, \frac{1}{4}$ ) x,y $+\frac{1}{4}$ , $\bar{y}$
(21) g( $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ ) x $+\frac{1}{4}$ ,y,x	(22) $\bar{4}^-$ $\frac{1}{4}, y, -\frac{1}{4}; \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$	(23) g( $\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}$ ) $\bar{x}+\frac{1}{4}$ ,y,x	(24) $\bar{4}^+$ $\frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0, \frac{1}{2}, \frac{1}{2})$ ;  $t(\frac{1}{2}, 0, \frac{1}{2})$ ; (2); (3); (5); (13)

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

(0,0,0)+ (0, $\frac{1}{2}$ , $\frac{1}{2}$ )+ ( $\frac{1}{2}$ ,0, $\frac{1}{2}$ )+ ( $\frac{1}{2}$ , $\frac{1}{2}$ ,0)+

Reflection conditions

 $h, k, l$  permutable

General:

96	$i$	1	(1) x,y,z	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{x}, y, \bar{z}$	(4) x, $\bar{y}, \bar{z}$
			(5) z,x,y	(6) z, $\bar{x}, \bar{y}$	(7) $\bar{z}, \bar{x}, y$	(8) $\bar{z}, x, \bar{y}$
			(9) y,z,x	(10) $\bar{y}, z, \bar{x}$	(11) y, $\bar{z}, \bar{x}$	(12) $\bar{y}, \bar{z}, x$
			(13) y,x,z	(14) $\bar{y}, \bar{x}, z$	(15) y, $\bar{x}, \bar{z}$	(16) $\bar{y}, x, \bar{z}$
			(17) x,z,y	(18) $\bar{x}, z, \bar{y}$	(19) $\bar{x}, \bar{z}, y$	(20) x, $\bar{z}, \bar{y}$
			(21) z,y,x	(22) z, $\bar{y}, \bar{x}$	(23) $\bar{z}, y, \bar{x}$	(24) $\bar{z}, \bar{y}, x$

 $hkl : h+k, h+l, k+l = 2n$  $OkI : k, l = 2n$  $hhl : h+l = 2n$  $h00 : h = 2n$ 

Special: no extra conditions

48	$h$	$. . m$	x,x,z	$\bar{x}, \bar{x}, z$	$\bar{x}, x, \bar{z}$	x, $\bar{x}, \bar{z}$	z,x,x	z, $\bar{x}, \bar{x}$
			$\bar{z}, \bar{x}, x$	$\bar{z}, x, \bar{x}$	x,z,x	$\bar{x}, z, \bar{x}$	x, $\bar{z}, \bar{x}$	$\bar{x}, \bar{z}, x$
24	$g$	2 . mm	x, $\frac{1}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$
24	$f$	2 . mm	x,0,0	$\bar{x}, 0, 0$	0,x,0	0, $\bar{x}, 0$	0,0,x	0,0, $\bar{x}$
16	$e$	. 3 m	x,x,x	$\bar{x}, \bar{x}, x$	$\bar{x}, x, \bar{x}$	x, $\bar{x}, \bar{x}$		
4	$d$	$\bar{4}3m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$					
4	$c$	$\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$					
4	$b$	$\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					
4	$a$	$\bar{4}3m$	0,0,0					

$P6_3mc$

$C_{6v}^4$

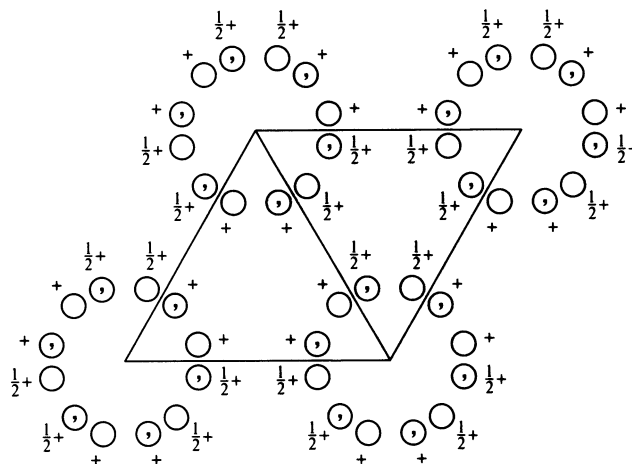
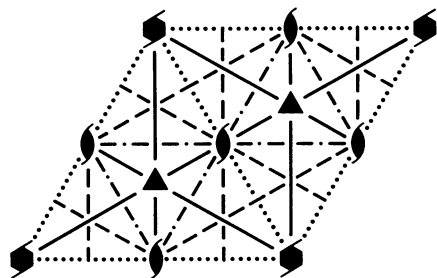
$6mm$

Hexagonal

No. 186

$P6_3mc$

Patterson symmetry  $P6/mmm$



Origin on  $3m1$  on  $6_3mc$

Asymmetric unit  $0 \leq x \leq \frac{2}{3}$ ;  $0 \leq y \leq \frac{1}{3}$ ;  $0 \leq z \leq 1$ ;  $x \leq (1+y)/2$ ;  $y \leq x/2$

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

Symmetry operations

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

**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>d</i> 1	(1) $x, y, z$	(2) $\bar{y}, x - y, z$	(3) $\bar{x} + y, \bar{x}, z$				$hh\bar{2}hl$ : $l = 2n$
	(4) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(5) $y, \bar{x} + y, z + \frac{1}{2}$	(6) $x - y, x, z + \frac{1}{2}$				$000l$ : $l = 2n$
	(7) $\bar{y}, \bar{x}, z$	(8) $\bar{x} + y, y, z$	(9) $x, x - y, z$				
	(10) $y, x, z + \frac{1}{2}$	(11) $x - y, \bar{y}, z + \frac{1}{2}$	(12) $\bar{x}, \bar{x} + y, z + \frac{1}{2}$				
							Special: as above, plus
6 <i>c</i> . <i>m</i> .	$x, \bar{x}, z$	$x, 2x, z$	$2\bar{x}, \bar{x}, z$	$\bar{x}, x, z + \frac{1}{2}$	$\bar{x}, 2\bar{x}, z + \frac{1}{2}$	$2x, x, z + \frac{1}{2}$	no extra conditions
2 <i>b</i> 3 <i>m</i> .	$\frac{1}{3}, \frac{2}{3}, z$	$\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}$					$hkl$ : $l = 2n$ or $h - k = 3n + 1$ or $h - k = 3n + 2$
2 <i>a</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$					$hkl$ : $l = 2n$

**Symmetry of special projections**

Along [001]  $p6mm$   
 $\mathbf{a}' = \mathbf{a}$     $\mathbf{b}' = \mathbf{b}$   
 Origin at 0, 0, z

Along [100]  $p1g1$   
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} + 2\mathbf{b})$     $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along [210]  $p1m1$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$     $\mathbf{b}' = \frac{1}{2}\mathbf{c}$   
 Origin at  $x, \frac{1}{2}x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $P6_311$ ( $P6_3, 173$ )	1; 2; 3; 4; 5; 6
	[2] $P31c$ (159)	1; 2; 3; 10; 11; 12
	[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9
	{ [3] $P2_1mc$ ( $Cmc2_1, 36$ )	1; 4; 7; 10
	{ [3] $P2_1mc$ ( $Cmc2_1, 36$ )	1; 4; 8; 11
	{ [3] $P2_1mc$ ( $Cmc2_1, 36$ )	1; 4; 9; 12

**IIa** none

**IIb** [3]  $H6_3mc$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) ( $P6_3cm, 185$ )

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $P6_3mc$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (186); [4]  $P6_3mc$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (186)

**Minimal non-isomorphic supergroups**

**I** [2]  $P6_3/mmc$  (194)

**II** [3]  $H6_3mc$  ( $P6_3cm, 185$ ); [2]  $P6mm$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (183)