

$Pn\bar{3}m$

O_h^4

$m\bar{3}m$

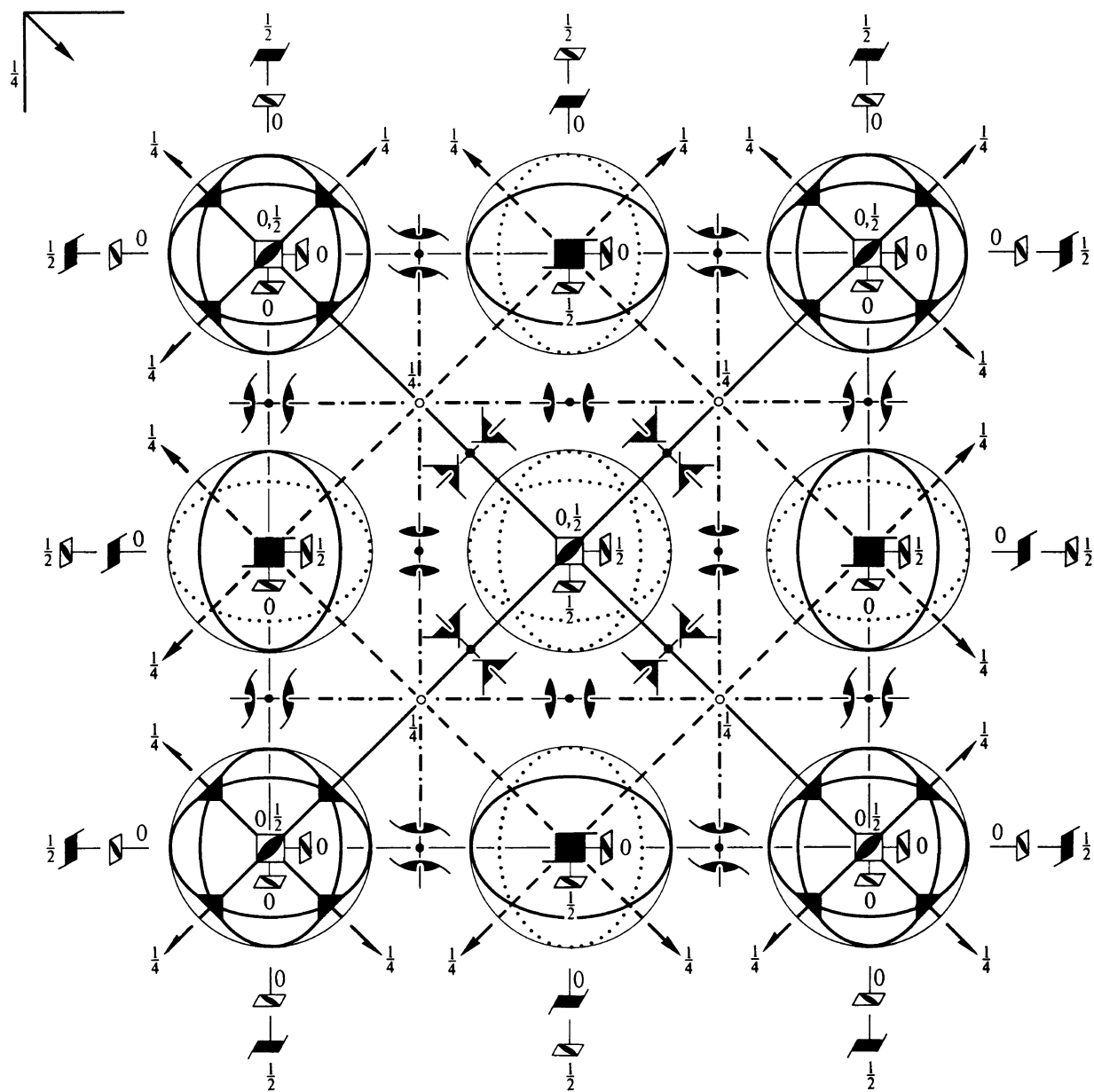
Cubic

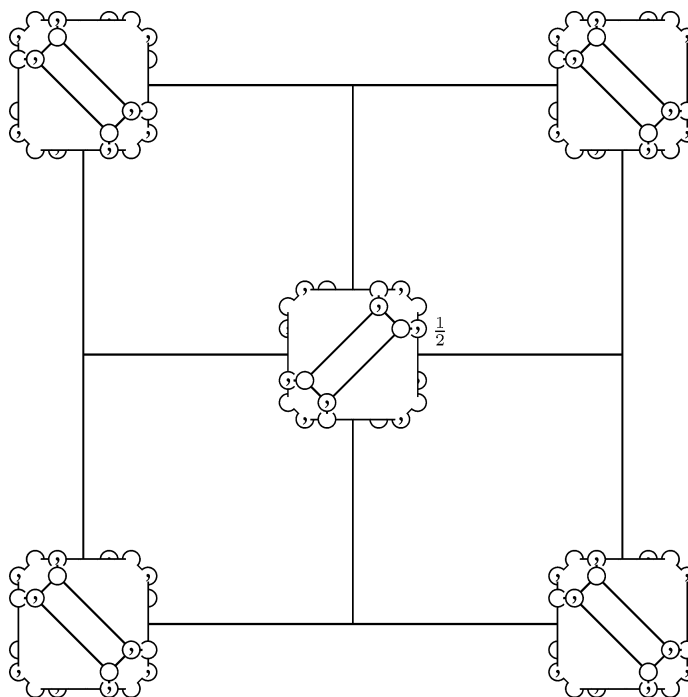
No. 224

$P4_2/n\bar{3}2/m$

Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1





Origin at $\bar{4}3m$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}m$)

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; -\frac{1}{4} \leq z \leq \frac{1}{4}; y \leq x; \max(x - \frac{1}{2}, -y) \leq z \leq \min(\frac{1}{2} - x, y)$

Vertices $0, 0, 0 \quad \frac{1}{2}, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, 0 \quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}$

Symmetry operations

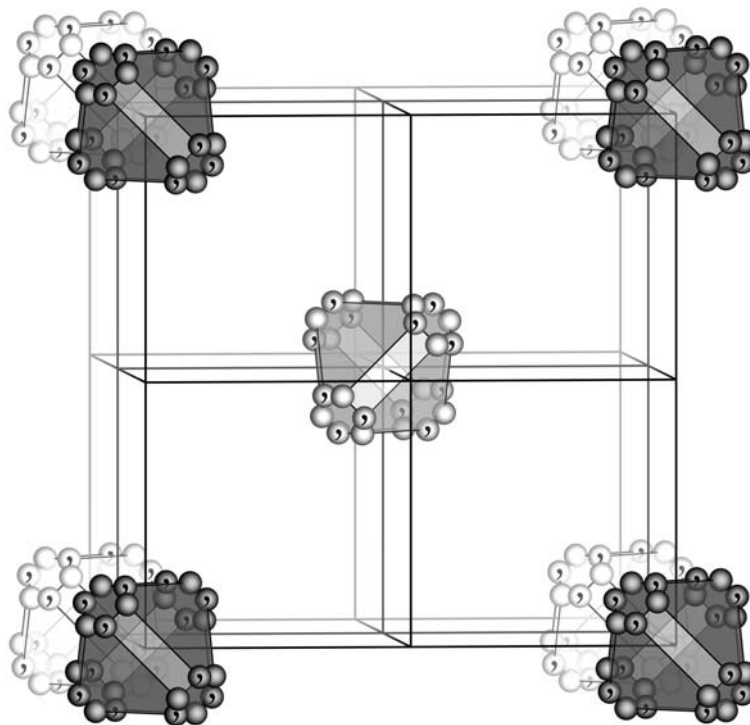
- | | | | |
|---|--|--|--|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 2 $0, y, 0$ | (4) 2 $x, 0, 0$ |
| (5) 3^+ x, x, x | (6) 3^+ \bar{x}, x, \bar{x} | (7) 3^+ x, \bar{x}, \bar{x} | (8) 3^+ \bar{x}, \bar{x}, x |
| (9) 3^- x, x, x | (10) 3^- x, \bar{x}, \bar{x} | (11) 3^- \bar{x}, \bar{x}, x | (12) 3^- \bar{x}, x, \bar{x} |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (14) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ | (15) $4^-(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ | (16) $4^+(0, 0, \frac{1}{2})$ $0, \frac{1}{2}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0)$ $x, \frac{1}{2}, 0$ | (18) $2(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, y$ | (19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{2}$ |
| (21) $4^+(0, \frac{1}{2}, 0)$ $\frac{1}{2}, y, 0$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, x$ | (23) $4^-(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{2}$ | (24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$ |
| (25) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (26) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (27) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (28) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ |
| (29) $\bar{3}^+$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (30) $\bar{3}^+$ $\bar{x} - 1, x + 1, \bar{x}; -\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ | (31) $\bar{3}^+$ $x, \bar{x} + 1, \bar{x}; \frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$ | (32) $\bar{3}^+$ $\bar{x} + 1, \bar{x}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$ |
| (33) $\bar{3}^-$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (34) $\bar{3}^-$ $x + 1, \bar{x} - 1, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$ | (35) $\bar{3}^-$ $\bar{x}, \bar{x} + 1, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ | (36) $\bar{3}^-$ $\bar{x} + 1, x, \bar{x}; \frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$ |
| (37) m x, \bar{x}, z | (38) m x, x, z | (39) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ | (40) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ |
| (41) $\bar{4}^-$ $x, 0, 0; 0, 0, 0$ | (42) m x, y, \bar{y} | (43) m x, y, y | (44) $\bar{4}^+$ $x, 0, 0; 0, 0, 0$ |
| (45) $\bar{4}^+$ $0, y, 0; 0, 0, 0$ | (46) m \bar{x}, y, x | (47) $\bar{4}^-$ $0, y, 0; 0, 0, 0$ | (48) m x, y, x |

ORIGIN CHOICE 1

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		
48 <i>l</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (25) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (29) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (33) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (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) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$ (26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (30) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$ (34) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ (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) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$ (27) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (35) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ (39) \bar{y}, x, \bar{z} (43) x, z, y (47) z, y, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (28) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (32) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (40) y, \bar{x}, \bar{z} (44) \bar{x}, z, \bar{y} (48) z, y, x	0 <i>kl</i> : $k + l = 2n$ h00: $h = 2n$		
					Special: as above, plus		
24 <i>k</i> . . <i>m</i>	x, x, z z, x, x x, z, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $z + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, z z, \bar{x}, \bar{x} \bar{x}, z, \bar{x} $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$ $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	\bar{x}, x, \bar{z} \bar{z}, \bar{x}, x x, \bar{z}, \bar{x} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	x, \bar{x}, \bar{z} \bar{z}, x, \bar{x} \bar{x}, \bar{z}, x $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	no extra conditions		
24 <i>j</i> . . 2	$\frac{1}{4}, y, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, \bar{y}$ $y, \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\frac{3}{4}, y + \frac{1}{2}, \bar{y}$ $y, \frac{1}{4}, y + \frac{1}{2}$	$\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $y, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \bar{y}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{1}{2}, y$ $y + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\bar{y}, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, y, \frac{1}{4}$	no extra conditions	
24 <i>i</i> . . 2	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $\frac{1}{4}, \bar{y} + \frac{1}{2}, y$ $\bar{y}, \frac{3}{4}, \bar{y} + \frac{1}{2}$	$\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\frac{3}{4}, y + \frac{1}{2}, y$ $\bar{y}, \frac{1}{4}, y + \frac{1}{2}$	$\frac{3}{4}, y, y + \frac{1}{2}$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, \bar{y}$ $\bar{y} + \frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$ $y + \frac{1}{2}, y, \frac{3}{4}$	$\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$ $y, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y}, \frac{1}{4}$	no extra conditions	
24 <i>h</i> 2 . .	$x, 0, \frac{1}{2}$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $0, x, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $x + \frac{1}{2}, 0, \frac{1}{2}$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$ $0, x + \frac{1}{2}, \frac{1}{2}$ $x, \frac{1}{2}, 0$	$0, \frac{1}{2}, x$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$ $\frac{1}{2}, 0, x$	$0, \frac{1}{2}, \bar{x}$ $0, \frac{1}{2}, x + \frac{1}{2}$ $\frac{1}{2}, 0, x + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x}$	<i>hkl</i> : $h + k + l = 2n$
12 <i>g</i> 2 . <i>mm</i>	$x, 0, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, x$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0, 0, \bar{x}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	<i>hkl</i> : $h + k + l = 2n$
12 <i>f</i> 2 . 22	$\frac{1}{4}, 0, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, 0, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{4}, 0$ $0, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{2}, \frac{3}{4}, 0$ $0, \frac{3}{4}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	<i>hkl</i> : $h + k + l = 2n$
8 <i>e</i> . 3 <i>m</i>	x, x, x $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, \bar{x}, x $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	\bar{x}, x, \bar{x} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$	x, \bar{x}, \bar{x} $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions		
6 <i>d</i> $\bar{4}2 . m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$	<i>hkl</i> : $h + k + l = 2n$
4 <i>c</i> . $\bar{3} m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$			<i>hkl</i> : $h + k, h + l, k + l = 2n$
4 <i>b</i> . $\bar{3} m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$			<i>hkl</i> : $h + k, h + l, k + l = 2n$
2 <i>a</i> $\bar{4}3 m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					<i>hkl</i> : $h + k + l = 2n$

**Symmetry of special projections**Along $[001]$ $p4mm$

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

Origin at $0, 0, z$ Along $[111]$ $p6mm$

$$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$$

Origin at x, x, x Along $[110]$ $p2mm$

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

Origin at $x, x, \frac{1}{4}$

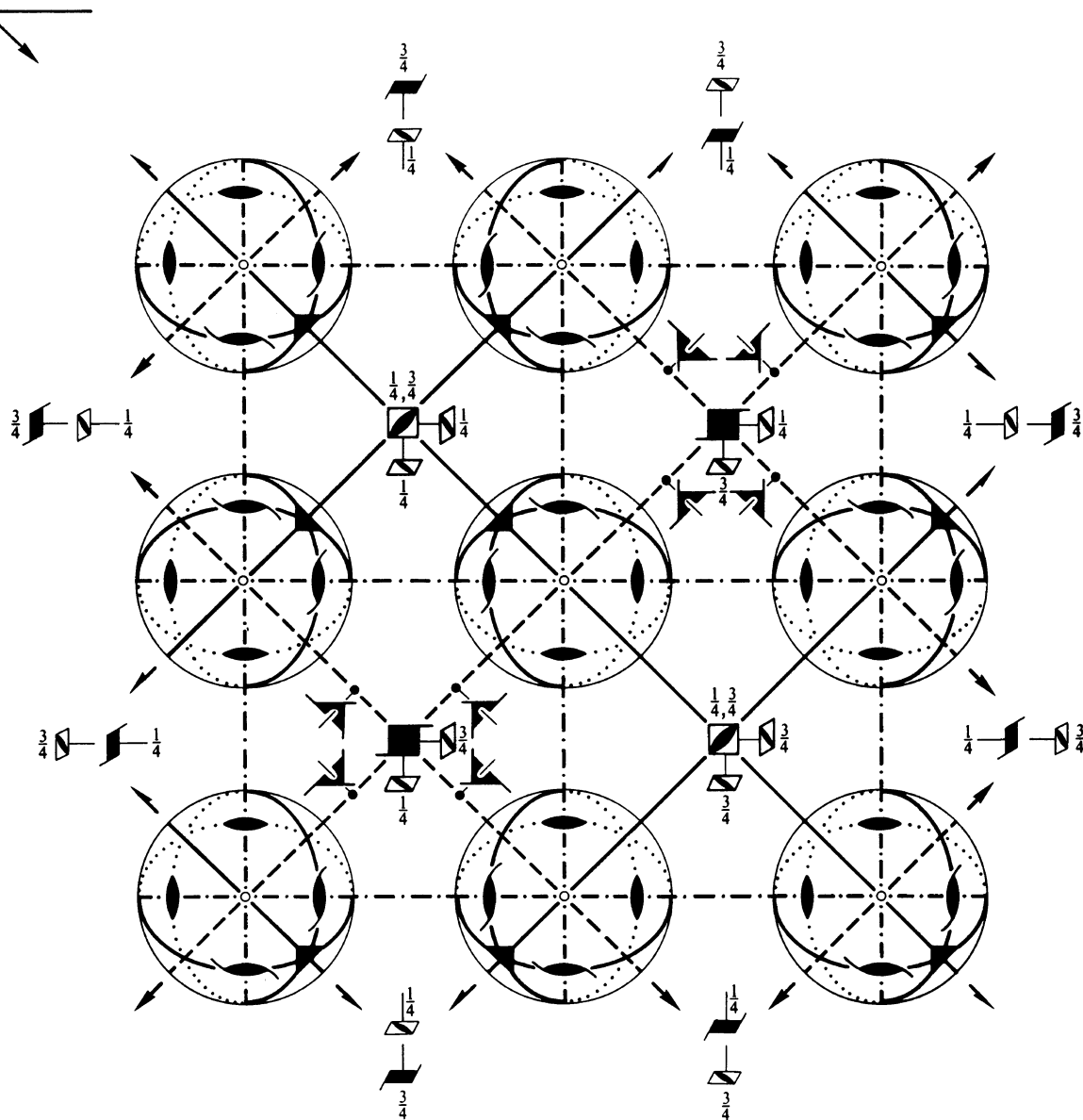
$Pn\bar{3}m$ O_h^4 $m\bar{3}m$

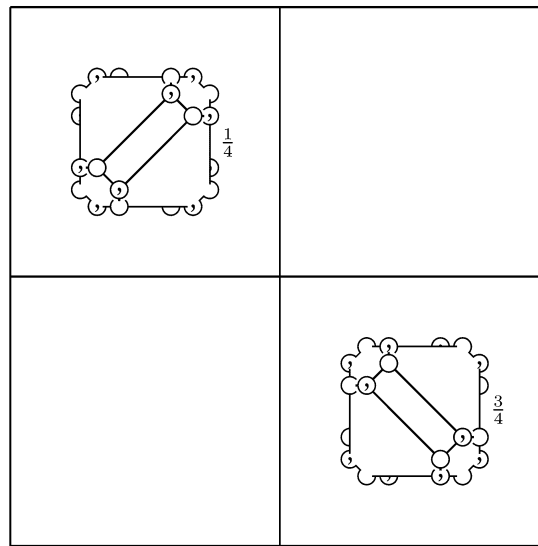
Cubic

No. 224

 $P 4_2/n \bar{3} 2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2





Origin at centre ($\bar{3}m$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{4}3m$

Asymmetric unit $\frac{1}{4} \leq x \leq \frac{3}{4}; \frac{1}{4} \leq y \leq \frac{3}{4}; 0 \leq z \leq \frac{1}{2}; y \leq x; \max(x - \frac{1}{2}, \frac{1}{2} - y) \leq z \leq \min(y, 1 - x)$

Vertices $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4} \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \quad \frac{1}{2}, \frac{1}{2}, 0$

Symmetry operations

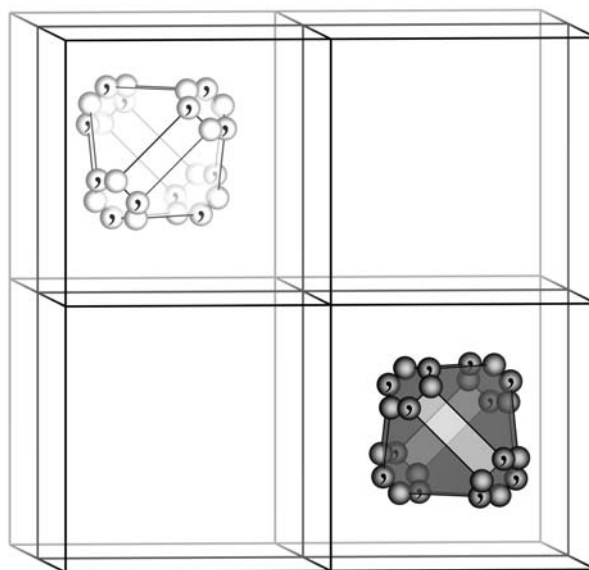
- | | | | |
|---|--|--|--|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $2 \frac{1}{4}, y, \frac{1}{4}$ | (4) $2 x, \frac{1}{4}, \frac{1}{4}$ |
| (5) $3^+ x, x, x$ | (6) $3^+ \bar{x}, x + \frac{1}{2}, \bar{x}$ | (7) $3^+ x + \frac{1}{2}, \bar{x}, \bar{x}$ | (8) $3^+ \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ |
| (9) $3^- x, x, x$ | (10) $3^- x + \frac{1}{2}, \bar{x}, \bar{x}$ | (11) $3^- \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ | (12) $3^- \bar{x}, x + \frac{1}{2}, \bar{x}$ |
| (13) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (14) $2 x, \bar{x}, 0$ | (15) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, -\frac{1}{4}, z$ | (16) $4^+(0, 0, \frac{1}{2}) -\frac{1}{4}, \frac{1}{4}, z$ |
| (17) $4^-(\frac{1}{2}, 0, 0) x, \frac{1}{4}, -\frac{1}{4}$ | (18) $2(0, \frac{1}{2}, \frac{1}{2}) 0, y, y$ | (19) $2 0, y, \bar{y}$ | (20) $4^+(\frac{1}{2}, 0, 0) x, -\frac{1}{4}, \frac{1}{4}$ |
| (21) $4^+(0, \frac{1}{2}, 0) \frac{1}{4}, y, -\frac{1}{4}$ | (22) $2(\frac{1}{2}, 0, \frac{1}{2}) x, 0, x$ | (23) $4^-(0, \frac{1}{2}, 0) -\frac{1}{4}, y, \frac{1}{4}$ | (24) $2 \bar{x}, 0, x$ |
| (25) $\bar{1} 0, 0, 0$ | (26) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (27) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ | (28) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ |
| (29) $\bar{3}^+ x, x, x; 0, 0, 0$ | (30) $\bar{3}^+ \bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$ | (31) $\bar{3}^+ x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$ | (32) $\bar{3}^+ \bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$ |
| (33) $\bar{3}^- x, x, x; 0, 0, 0$ | (34) $\bar{3}^- x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$ | (35) $\bar{3}^- \bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$ | (36) $\bar{3}^- \bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$ |
| (37) $m x + \frac{1}{2}, \bar{x}, z$ | (38) $m x, x, z$ | (39) $\bar{4}^- \frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (40) $\bar{4}^+ \frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (41) $\bar{4}^- x, \frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (42) $m x, y + \frac{1}{2}, \bar{y}$ | (43) $m x, y, y$ | (44) $\bar{4}^+ x, \frac{1}{4}, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (45) $\bar{4}^+ \frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (46) $m \bar{x} + \frac{1}{2}, y, x$ | (47) $\bar{4}^- \frac{1}{4}, y, \frac{1}{4}; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (48) $m x, y, x$ |

ORIGIN CHOICE 2

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
48 l 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (5) z, x, y (6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$ (8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (9) y, z, x (10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ (11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ (13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (14) $\bar{y}, \bar{x}, \bar{z}$ (15) $y + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ (16) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{2}$ (17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y}$ (18) $\bar{x}, z + \frac{1}{2}, y + \frac{1}{2}$ (19) $\bar{x}, \bar{z}, \bar{y}$ (20) $x + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$ (21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x}$ (22) $z + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$ (23) $\bar{z}, y + \frac{1}{2}, x + \frac{1}{2}$ (24) $\bar{z}, \bar{y}, \bar{x}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (27) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (28) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (30) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$ (31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (32) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (34) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (35) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (38) y, x, z (39) $\bar{y} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$ (40) $y, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$ (42) $x, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (43) x, z, y (44) $\bar{x} + \frac{1}{2}, z, \bar{y} + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x$ (46) $\bar{z} + \frac{1}{2}, y, \bar{x} + \frac{1}{2}$ (47) $z, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (48) z, y, x	Okl: $k + l = 2n$ h00: $h = 2n$
24 k $\dots m$	x, x, z $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ z, x, x $z, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $\bar{z} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ x, z, x $\bar{x} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ $x, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ $\bar{x}, \bar{x}, \bar{z}$ $x + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ $\bar{x}, z + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x}, \bar{z}, \bar{x}$ $x + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ $z + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $z + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{z}, x + \frac{1}{2}, x + \frac{1}{2}$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
24 j $\dots 2$	$\frac{1}{2}, y, \bar{y}$ $0, \bar{y} + \frac{1}{2}, \bar{y}$ $0, y, y + \frac{1}{2}$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, y + \frac{1}{2}$ $\bar{y}, \frac{1}{2}, y$ $\bar{y}, 0, \bar{y} + \frac{1}{2}$ $y + \frac{1}{2}, 0, y$ $y + \frac{1}{2}, \frac{1}{2}, \bar{y} + \frac{1}{2}$ $y, \bar{y}, \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y}, 0$ $y, y + \frac{1}{2}, 0$ $\bar{y} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{y}, y$ $0, y + \frac{1}{2}, y$ $0, \bar{y}, \bar{y} + \frac{1}{2}$ $\frac{1}{2}, y + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $y, \frac{1}{2}, \bar{y}$ $y, 0, y + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, 0, \bar{y}$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}$ $\bar{y}, y, \frac{1}{2}$ $y + \frac{1}{2}, y, 0$ $\bar{y}, \bar{y} + \frac{1}{2}, 0$ $y + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
24 i $\dots 2$	$\frac{1}{2}, y, y + \frac{1}{2}$ $0, \bar{y} + \frac{1}{2}, y + \frac{1}{2}$ $0, y, \bar{y}$ $\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{y}$ $y + \frac{1}{2}, \frac{1}{2}, y$ $y + \frac{1}{2}, 0, \bar{y} + \frac{1}{2}$ $\bar{y}, 0, y$ $\bar{y}, \frac{1}{2}, \bar{y} + \frac{1}{2}$ $y, y + \frac{1}{2}, \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y + \frac{1}{2}, 0$ $y, \bar{y}, 0$ $\bar{y} + \frac{1}{2}, \bar{y}, \frac{1}{2}$ $\frac{1}{2}, \bar{y}, \bar{y} + \frac{1}{2}$ $0, y + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $0, \bar{y}, y$ $\frac{1}{2}, y + \frac{1}{2}, y$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{y}$ $\bar{y} + \frac{1}{2}, 0, y + \frac{1}{2}$ $y, 0, \bar{y}$ $y, \frac{1}{2}, y + \frac{1}{2}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{2}$ $y + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$ $\bar{y}, y, 0$ $y + \frac{1}{2}, y, \frac{1}{2}$	no extra conditions
24 h $2\dots$	$x, \frac{1}{4}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, x$ $\frac{1}{4}, \frac{3}{4}, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\bar{x}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, x, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $x, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$	$hkl: h + k + l = 2n$
12 g $2.mmm$	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$ $\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}$	$hkl: h + k + l = 2n$
12 f 2.22	$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $0, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, 0, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $0, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, 0, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, 0$	$hkl: h + k + l = 2n$
8 e $.3m$	x, x, x $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $\bar{x}, \bar{x}, \bar{x}$ $x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$	no extra conditions
6 d $\bar{4}2.m$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl: h + k + l = 2n$
4 c $.3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$ $0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl: h + k, h + l, k + l = 2n$
4 b $.3m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k, h + l, k + l = 2n$
2 a $\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: h + k + l = 2n$

**Symmetry of special projections**

Along $[001]$ $p4mm$
 $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$
 Origin at $\frac{1}{4}, \frac{1}{4}, z$

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 $x, x, 0$