

$I\bar{m}\bar{3}m$

$O_h^9$

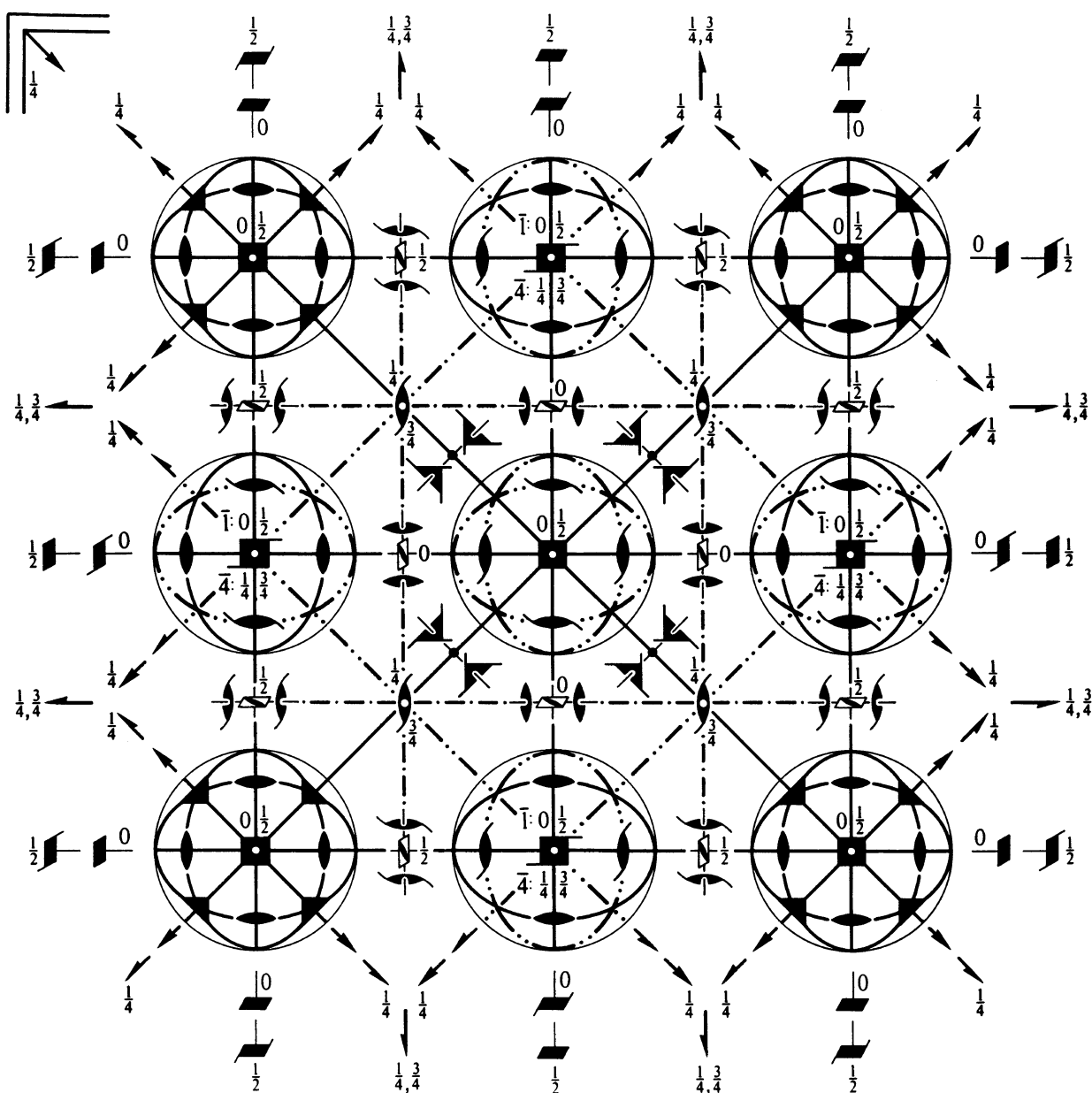
$m\bar{3}m$

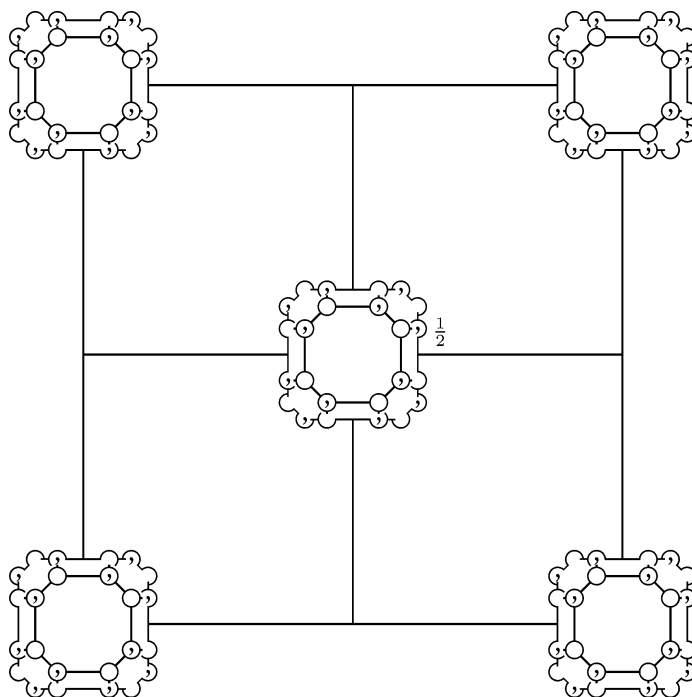
Cubic

No. 229

$I 4/m \bar{3} 2/m$

Patterson symmetry  $I\bar{m}\bar{3}m$





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

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

**Vertices**  $0,0,0$   $\frac{1}{2},0,0$   $\frac{1}{2},\frac{1}{2},0$   $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

### 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) $3^+$ $x,x,x$               | (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 $x,x,0$                  | (14) 2 $x,\bar{x},0$                        | (15) $4^-$ $0,0,z$                          | (16) $4^+$ $0,0,z$                          |
| (17) $4^-$ $x,0,0$              | (18) 2 $0,y,y$                              | (19) 2 $0,y,\bar{y}$                        | (20) $4^+$ $x,0,0$                          |
| (21) $4^+$ $0,y,0$              | (22) 2 $x,0,x$                              | (23) $4^-$ $0,y,0$                          | (24) 2 $\bar{x},0,x$                        |
| (25) $\bar{1}$ $0,0,0$          | (26) $m$ $x,y,0$                            | (27) $m$ $x,0,z$                            | (28) $m$ $0,y,z$                            |
| (29) $\bar{3}^+$ $x,x,x; 0,0,0$ | (30) $\bar{3}^+$ $\bar{x},x,\bar{x}; 0,0,0$ | (31) $\bar{3}^+$ $x,\bar{x},\bar{x}; 0,0,0$ | (32) $\bar{3}^+$ $\bar{x},\bar{x},x; 0,0,0$ |
| (33) $\bar{3}^-$ $x,x,x; 0,0,0$ | (34) $\bar{3}^-$ $x,\bar{x},\bar{x}; 0,0,0$ | (35) $\bar{3}^-$ $\bar{x},\bar{x},x; 0,0,0$ | (36) $\bar{3}^-$ $\bar{x},x,\bar{x}; 0,0,0$ |
| (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) $m$ $x,y,x$                            |

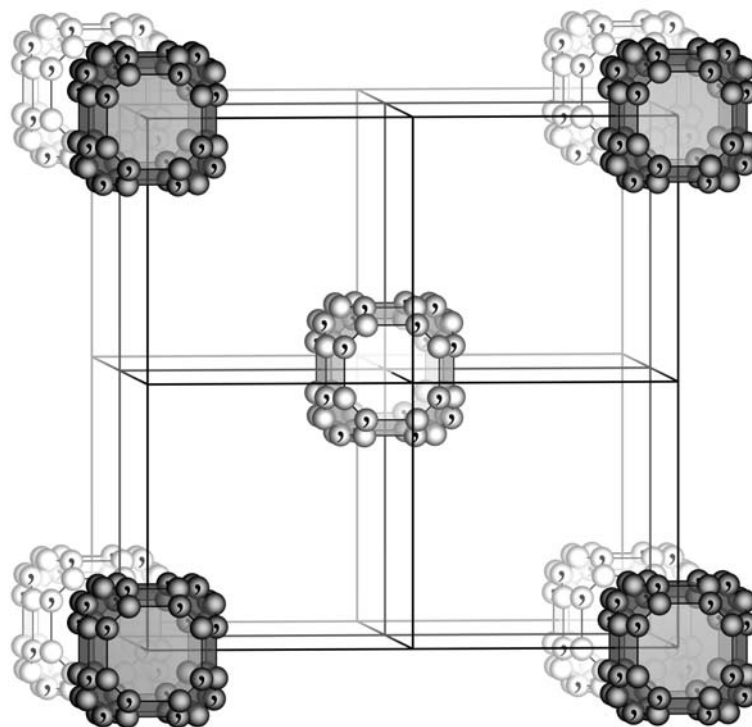
For  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$  set

- |   |  |  |  |
|---|--|--|--|
| (1) $i(\frac{1}{2},\frac{1}{2},\frac{1}{2})$                  | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$   | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$   | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$   |
| (5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,x,x$        | (6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$  | (7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$  | (8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$  |
| (9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,x,x$        | (10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$ | (11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$ | (12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$ |
| (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) $c$ $x+\frac{1}{2},\bar{x},z$                            | (38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,x,z$  | (39) $\bar{4}^-$ $0,\frac{1}{2},z; 0,\frac{1}{2},\frac{1}{4}$                                | (40) $\bar{4}^+$ $\frac{1}{2},0,z; \frac{1}{2},0,\frac{1}{4}$                                |
| (41) $\bar{4}^-$ $x,0,\frac{1}{2}; \frac{1}{4},0,\frac{1}{2}$ | (42) $a$ $x,y+\frac{1}{2},\bar{y}$   | (43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,y,y$  | (44) $\bar{4}^+$ $x,\frac{1}{2},0; \frac{1}{4},\frac{1}{2},0$                                |
| (45) $\bar{4}^+$ $0,y,\frac{1}{2}; 0,\frac{1}{4},\frac{1}{2}$ | (46) $b$ $\bar{x}+\frac{1}{2},y,x$   | (47) $\bar{4}^-$ $\frac{1}{2},y,0; \frac{1}{2},\frac{1}{4},0$                                | (48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $x,y,x$  |

**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	$l$ 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) $z, y, x$	Reflection conditions $h, k, l$ permutable General: $hkl: h + k + l = 2n$ $OkI: k + l = 2n$ $hhl: l = 2n$ $h00: h = 2n$		
48	$k$ $..m$	$x, x, z$ $\bar{z}, \bar{x}, x$ $x, x, \bar{z}$ $\bar{x}, \bar{z}, \bar{x}$	$\bar{x}, \bar{x}, z$ $\bar{z}, x, \bar{x}$ $\bar{x}, \bar{x}, \bar{z}$ $x, \bar{z}, x$	$\bar{x}, x, \bar{z}$ $x, z, x$ $x, \bar{x}, z$ $z, x, \bar{x}$	$x, \bar{x}, \bar{z}$ $\bar{x}, z, \bar{x}$ $\bar{x}, x, z$ $z, \bar{x}, x$	$z, x, x$ $x, \bar{z}, \bar{x}$ $x, z, \bar{x}$ $\bar{z}, x, x$	$z, \bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$ $\bar{x}, z, x$ $\bar{z}, \bar{x}, \bar{x}$	Special: as above, plus no extra conditions
48	$j$ $m..$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions
48	$i$ $..2$	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, y$ $y, y + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$	no extra conditions		
24	$h$ $m.m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions
24	$g$ $mm2..$	$x, 0, \frac{1}{2}$ $0, x, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $x, \frac{1}{2}, 0$	$\frac{1}{2}, \bar{x}, 0$ $\bar{x}, \frac{1}{2}, 0$	$0, \frac{1}{2}, x$ $\frac{1}{2}, 0, \bar{x}$	$0, \frac{1}{2}, \bar{x}$ $\frac{1}{2}, 0, x$	no extra conditions
16	$f$ $.3m$	$x, x, x$ $x, x, \bar{x}$	$\bar{x}, \bar{x}, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x}, x, \bar{x}$ $x, \bar{x}, x$	$x, \bar{x}, \bar{x}$ $\bar{x}, x, x$	no extra conditions		
12	$e$ $4m.m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
12	$d$ $\bar{4}m.2$	$\frac{1}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{3}{4}, 0$	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	no extra conditions
8	$c$ $.\bar{3}m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl: k, l = 2n$		
6	$b$ $4/m.m.m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	no extra conditions			
2	$a$ $m\bar{3}m$	$0, 0, 0$	no extra conditions					

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

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

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  $[110]$   $p2mm$ 

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

Origin at  $x, x, 0$