

$Pm\bar{3}n$

$O_h^3$

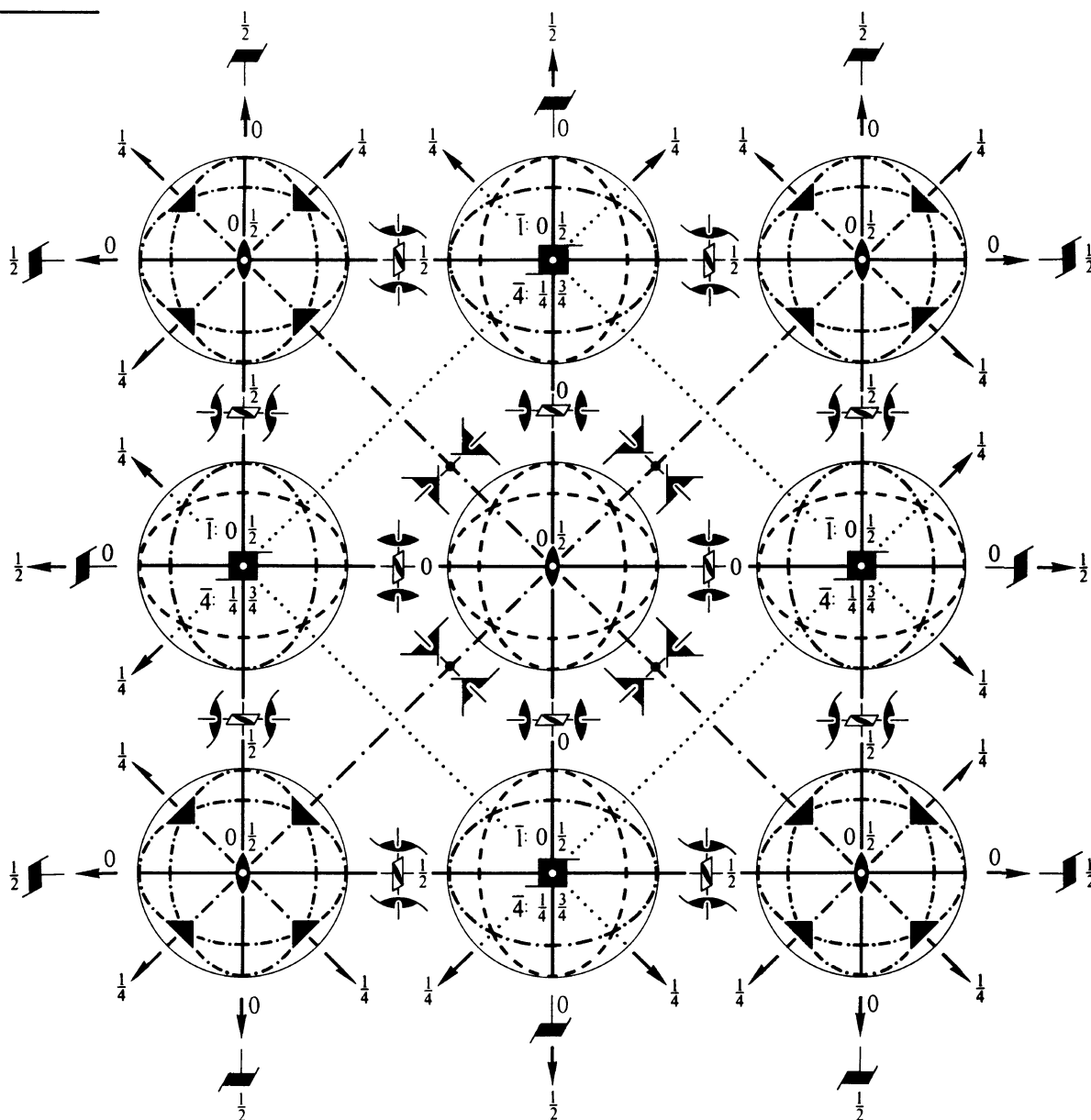
$m\bar{3}m$

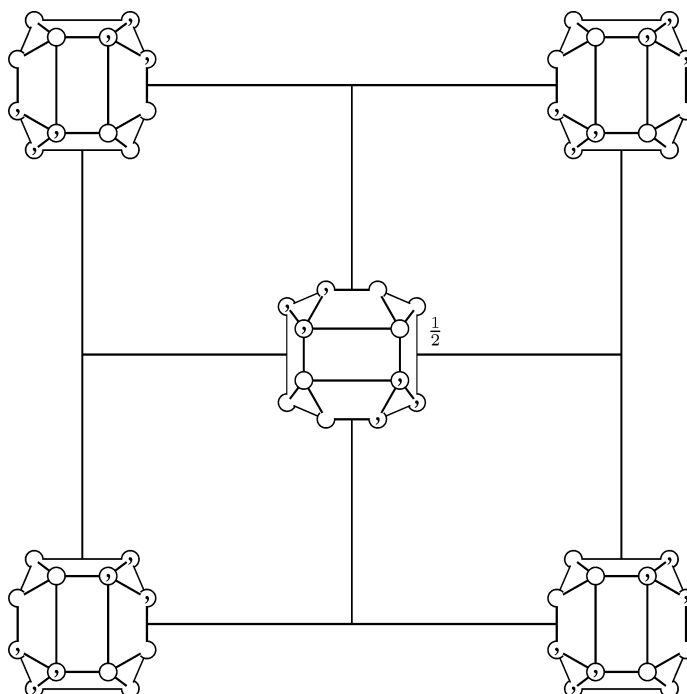
Cubic

No. 223

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

Patterson symmetry  $Pm\bar{3}m$





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

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

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

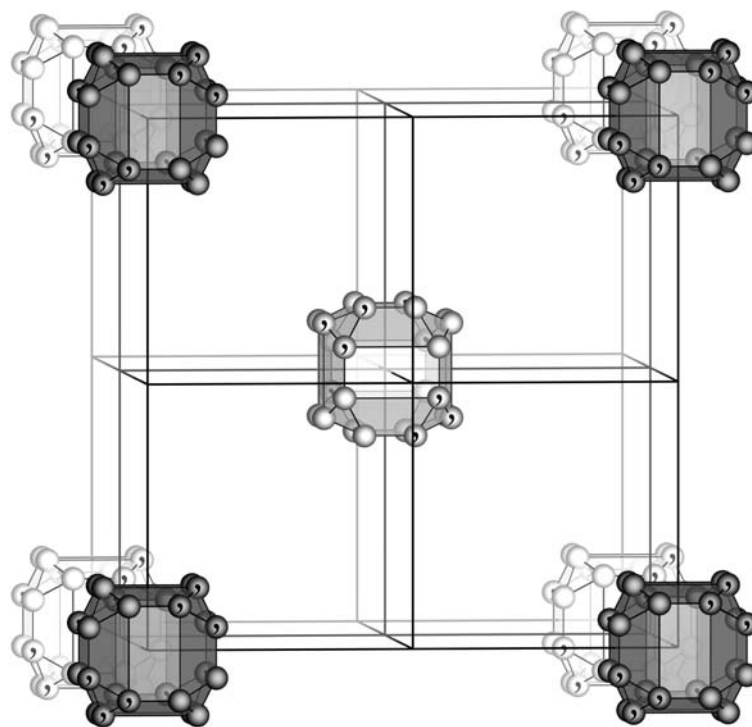
### Symmetry operations

- |  |   |  |  |
|--|---|--|--|
| (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) $\bar{1}$ $0, 0, 0$   | (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) $c$ $x + \frac{1}{2}, \bar{x}, z$                               | (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);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3); (5); (13); (25)

**Positions**

		Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions	
							$h, k, l$ permutable	
							General:	
48	$l$	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) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ (45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(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) $x, y, \bar{z}$ (30) $\bar{z}, x, y$ (34) $y, \bar{z}, x$ (38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (42) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (46) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(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) $x, \bar{y}, z$ (31) $z, x, \bar{y}$ (35) $\bar{y}, z, x$ (39) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (47) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(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) $\bar{x}, y, z$ (32) $z, \bar{x}, y$ (36) $y, z, \bar{x}$ (40) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (44) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	$hkl: l = 2n$ $h00: h = 2n$	
24	$k$	$m..$	$0, y, z$ $z, 0, y$ $y, z, 0$ $y + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, z$ $z, 0, \bar{y}$ $\bar{y}, z, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	$0, y, \bar{z}$ $\bar{z}, 0, y$ $y, \bar{z}, 0$ $y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$0, \bar{y}, \bar{z}$ $\bar{z}, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $\bar{y} + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$ $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	Special: as above, plus no extra conditions	
24	$j$	$..2$	$\frac{1}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, y$ $y, y + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{1}{4}$	$\frac{3}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, y$ $y, \bar{y} + \frac{1}{2}, \frac{3}{4}$ $\frac{1}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y}$ $\bar{y}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, y, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y$ $y, y + \frac{1}{2}, \frac{3}{4}$	$hkl: h = 2n$	
16	$i$	$.3.$	$x, x, x$ $\bar{x}, x, \bar{x}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{x}$ $x, \bar{x}, x$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\bar{x}, \bar{x}, x$ $x, \bar{x}, \bar{x}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ $x, x, \bar{x}$ $\bar{x}, x, x$ $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$			$hkl: h + k + l = 2n$	
12	$h$	$mm2..$	$x, \frac{1}{2}, 0$ $\frac{1}{2}, 0, x$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$ $0, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \bar{x} + \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $0, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, x + \frac{1}{2}$	$hkl: h = 2n$	
12	$g$	$mm2..$	$x, 0, \frac{1}{2}$ $0, \frac{1}{2}, x$ $x + \frac{1}{2}, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \bar{x}$ $\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, x, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$\frac{1}{2}, \bar{x}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $0, \frac{1}{2}, x + \frac{1}{2}$	$hkl: h = 2n$	
12	$f$	$mm2..$	$x, 0, 0$ $0, 0, x$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $0, 0, \bar{x}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, x, 0$ $\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{x} + \frac{1}{2}$	$0, \bar{x}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}$	$hkl: h + k + l = 2n$	
8	$e$	$.32$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h, k, l = 2n$	
6	$d$	$\bar{4}m.2$	$\frac{1}{4}, \frac{1}{2}, 0$	$\frac{3}{4}, \frac{1}{2}, 0$	$0, \frac{1}{4}, \frac{1}{2}$	$0, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{4}$	} $hkl: h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$
6	$c$	$\bar{4}m.2$	$\frac{1}{4}, 0, \frac{1}{2}$	$\frac{3}{4}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{4}, 0$	$\frac{1}{2}, \frac{3}{4}, 0$	$0, \frac{1}{2}, \frac{1}{4}$	
6	$b$	$mmm..$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	
2	$a$	$m\bar{3}.$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				$hkl: h + k + l = 2n$

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

$$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$$

Origin at  $0, \frac{1}{2}, z$ Along  $[111]$   $p6mm$ 

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

Origin at  $x, x, x$ 

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

Along  $[110]$   $p2mm$ 

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

Origin at  $x, x, 0$ 

$$\mathbf{b}' = \frac{1}{2}\mathbf{c}$$