

$Pn\bar{3}$

T_h^2

$m\bar{3}$

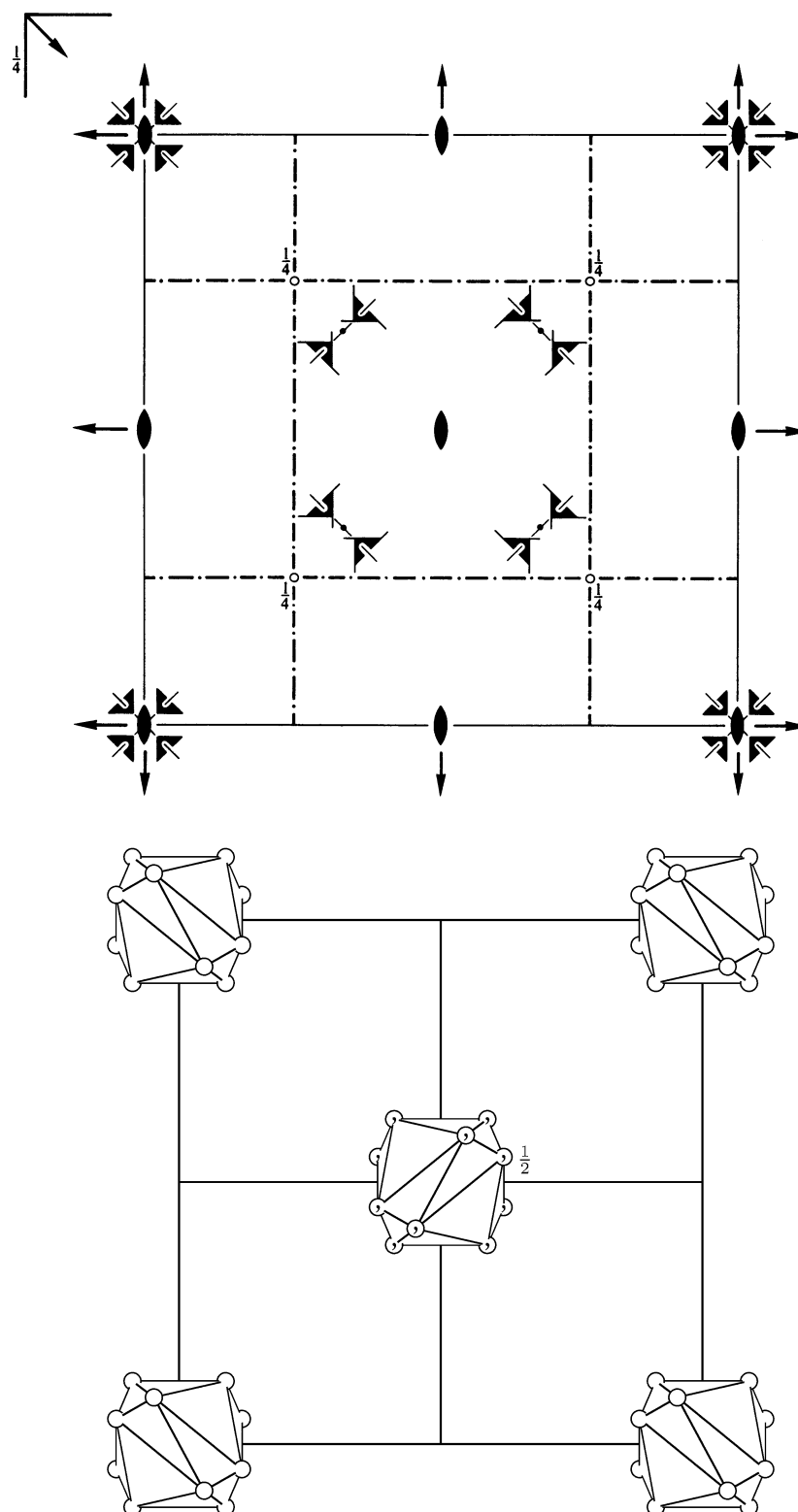
Cubic

No. 201

$P2/n\bar{3}$

Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 1



Origin at $2\bar{3}$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}$)

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

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) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $n(\frac{1}{2},\frac{1}{2},0)$ x,y, $\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2})$ x, $\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(17) 3 ⁺ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) 3 ⁺ $\bar{x}-1,x+1,\bar{x}; -\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(19) 3 ⁺ x, $\bar{x}+1,\bar{x}; \frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(20) 3 ⁺ $\bar{x}+1,\bar{x},x; \frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(21) 3 ⁻ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) 3 ⁻ x+1, $\bar{x}-1,\bar{x}; \frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(23) 3 ⁻ $\bar{x},\bar{x}+1,x; -\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(24) 3 ⁻ $\bar{x}+1,x,\bar{x}; \frac{3}{4},\frac{1}{4},-\frac{1}{4}$

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

 h, k, l cyclically permutable

General:

24	h	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	OkI: $k+l=2n$
			(13) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(17) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(21) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	h00: $h=2n$

Special: as above, plus

12	g	2..	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	0,x, $\frac{1}{2}$	0, $\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$	
12	f	2..	x,0,0	$\bar{x},0,0$	0,x,0	0, $\bar{x},0$	0,0,x	0,0, \bar{x}	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
8	e	.3.	x,x,x	\bar{x},\bar{x},x					no extra conditions
			\bar{x},x,\bar{x}	x, \bar{x},\bar{x}					
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
6	d	222..	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
4	c	. $\bar{3}$.	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl: $h+k,h+l,k+l=2n$
4	b	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k,h+l,k+l=2n$
2	a	23.	0,0,0	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at 0,0,z

Along [111] $p6$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$

Origin at x,x,x

 $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at x,x, $\frac{1}{4}$

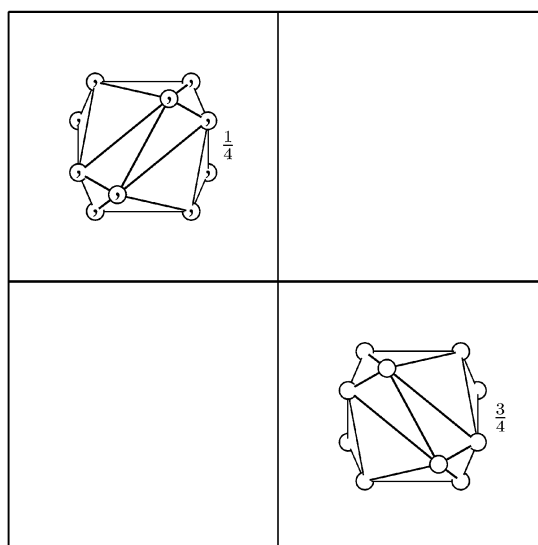
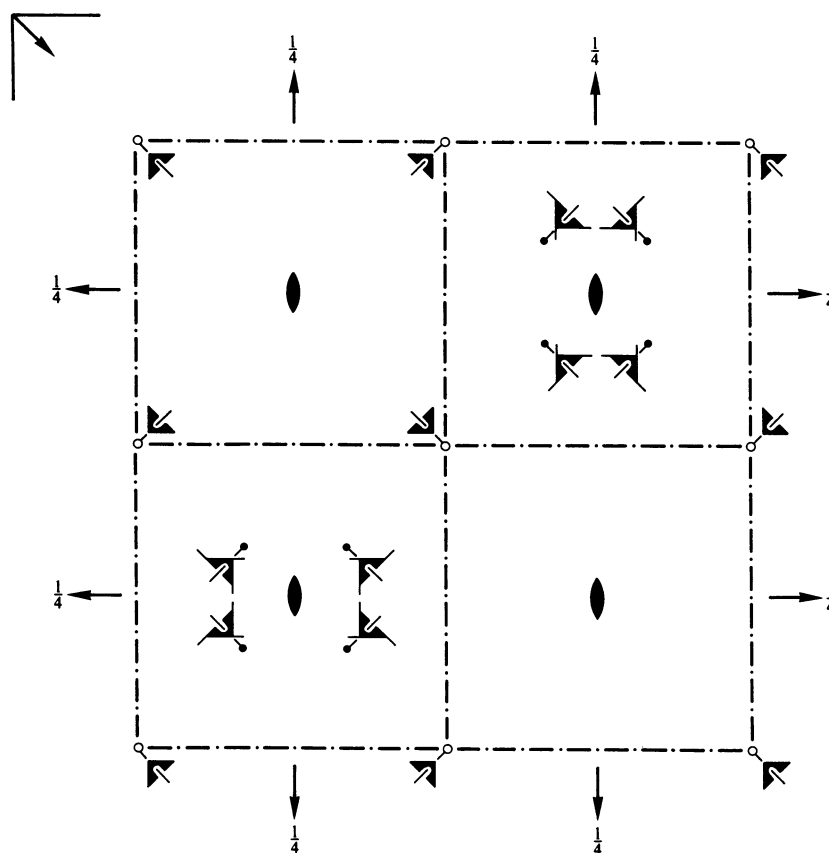
$Pn\bar{3}$ T_h^2 $m\bar{3}$

Cubic

No. 201

 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 2



Origin at centre ($\bar{3}$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from 23

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

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) $\bar{1}$ 0,0,0	(14) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$	(15) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, 0, z$	(16) $n(0, \frac{1}{2}, \frac{1}{2})$ $0, y, z$
(17) $\bar{3}^+$ $x, x, x; 0, 0, 0$	(18) $\bar{3}^+$ $\bar{x} - 1, x + \frac{1}{2}, \bar{x}; -\frac{1}{2}, 0, \frac{1}{2}$	(19) $\bar{3}^+$ $x - \frac{1}{2}, \bar{x} + 1, \bar{x}; 0, \frac{1}{2}, -\frac{1}{2}$	(20) $\bar{3}^+$ $\bar{x} + \frac{1}{2}, \bar{x} - \frac{1}{2}, x; \frac{1}{2}, -\frac{1}{2}, 0$
(21) $\bar{3}^-$ $x, x, x; 0, 0, 0$	(22) $\bar{3}^-$ $x + \frac{1}{2}, \bar{x} - 1, \bar{x}; 0, -\frac{1}{2}, \frac{1}{2}$	(23) $\bar{3}^-$ $\bar{x} - \frac{1}{2}, \bar{x} + \frac{1}{2}, x; -\frac{1}{2}, \frac{1}{2}, 0$	(24) $\bar{3}^-$ $\bar{x} + 1, x - \frac{1}{2}, \bar{x}; \frac{1}{2}, 0, -\frac{1}{2}$

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

 h, k, l cyclically permutable

General:

24	h	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) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0kl: k + l = 2n$ $h00: h = 2n$
			(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) $\bar{x}, \bar{y}, \bar{z}$	(14) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(15) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(16) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	
			(17) $\bar{z}, \bar{x}, \bar{y}$	(18) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$	(19) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	(20) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$	
			(21) $\bar{y}, \bar{z}, \bar{x}$	(22) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$	(23) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$	(24) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$	

Special: as above, plus

12	g	2..	$x, \frac{3}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, x$	$\frac{3}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$	$hkl: h + k + l = 2n$
			$\bar{x}, \frac{1}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \bar{x}, \frac{1}{4}$	$\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \bar{x}$	$\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}$	
12	f	2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, x, \frac{1}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$	$\frac{1}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$	$hkl: h + k + l = 2n$
			$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \bar{x}$	$\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}$	
8	e	.3.	x, x, x	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$	$\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	no extra conditions		
			$\bar{x}, \bar{x}, \bar{x}$	$x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$	$x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$			
6	d	222..	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl: h + k + l = 2n$
4	c	. $\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl: h + k, h + l, k + l = 2n$		
4	b	. $\bar{3}$.	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl: h + k, h + l, k + l = 2n$		
2	a	23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$				$hkl: h + k + l = 2n$	

Symmetry of special projections

Along [001] $c2mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $\frac{1}{4}, \frac{1}{4}, z$ Along [111] $p6$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ Origin at x, x, x $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$