

$P4_2/nnm$
 D_{4h}^{12}
 $4/mmm$

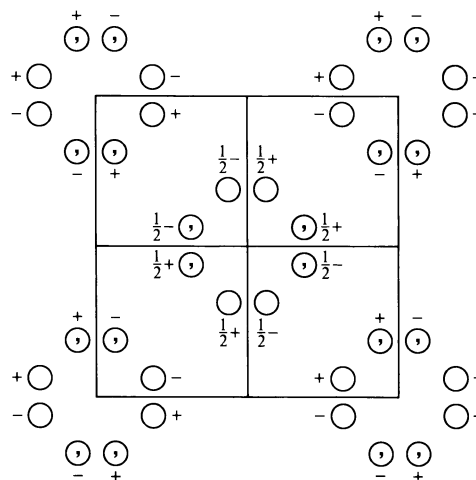
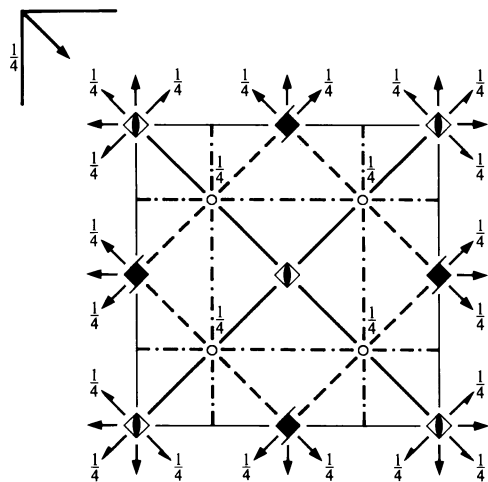
Tetragonal

No. 134

 $P 4_2/n 2/n 2/m$

 Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1


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

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{4}; x \leq y; y \leq 1-x$
Symmetry operations

- | | | | |
|---------------------------------------------------------|---------------------------------------------------------|--------------------------------------------------------|------------------------------------------------|
| (1) 1 | (2) 2 $0, 0, z$ | (3) $4^+(0, 0, \frac{1}{2}) 0, \frac{1}{2}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{2}, 0, z$ |
| (5) 2 $0, y, 0$ | (6) 2 $x, 0, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, \frac{1}{4}$ | (11) $\bar{4}^+ 0, 0, z; 0, 0, 0$ | (12) $\bar{4}^- 0, 0, z; 0, 0, 0$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2}) x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2}) \frac{1}{4}, y, z$ | (15) $m x, \bar{x}, z$ | (16) $m x, x, z$ |

Maximal non-isomorphic subgroups

- | | | |
|----------|---------------------------------|----------------------------|
| I | [2] $P\bar{4}n2$ (118) | 1; 2; 7; 8; 11; 12; 13; 14 |
| | [2] $P\bar{4}2m$ (111) | 1; 2; 5; 6; 11; 12; 15; 16 |
| | [2] $P4_2nm$ (102) | 1; 2; 3; 4; 13; 14; 15; 16 |
| | [2] $P4_222$ (93) | 1; 2; 3; 4; 5; 6; 7; 8 |
| | [2] $P4_2/n11$ ($P4_2/n$, 86) | 1; 2; 3; 4; 9; 10; 11; 12 |
| | [2] $P2/n12/m$ ($Cmme$, 67) | 1; 2; 7; 8; 9; 10; 15; 16 |
| | [2] $P2/n2/n1$ ($Pnmm$, 48) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

IIb [2] $F4_1/ddc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/amd$, 141)

Maximal isomorphic subgroups of lowest index
IIc [3] $P4_2/nnm$ ($\mathbf{c}' = 3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (134)

Minimal non-isomorphic supergroups
I [3] $Pn\bar{3}m$ (224)

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
16	n 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	$hk0 : h + k = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
					Special: as above, plus	
8	m $\dots m$	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	l $\dots 2$	$x, x + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$	$hkl : h + k = 2n$
8	k $\dots 2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{1}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, x, \frac{1}{4}$	$\bar{x}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl : h + k = 2n$
8	j $\dots 2$	$x, 0, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, \frac{1}{2}$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, x + \frac{1}{2}, 0$ $0, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $0, x, \frac{1}{2}$	$hkl : h + k + l = 2n$
8	i $\dots 2$	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $0, \bar{x}, 0$	$\frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $0, x, 0$	$hkl : h + k + l = 2n$
8	h $2 \dots$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
4	g $2 \dots mm$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	f $\dots 2/m$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	e $\dots 2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k, h + l, k + l = 2n$
4	d $2 \dots 22$	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4	c $2 \dots 22$	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
2	b $\bar{4}2m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k + l = 2n$
2	a $\bar{4}2m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

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

Origin at $0, 0, z$

Along $[100]$ $c2mm$

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

Origin at $x, 0, 0$

Along $[110]$ $p2mm$

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

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

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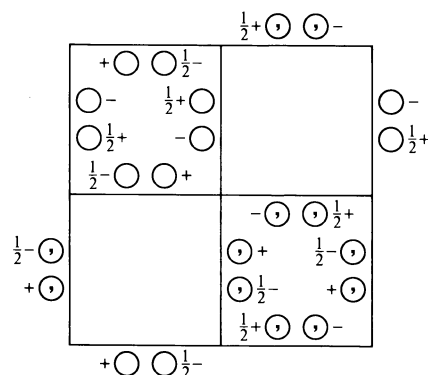
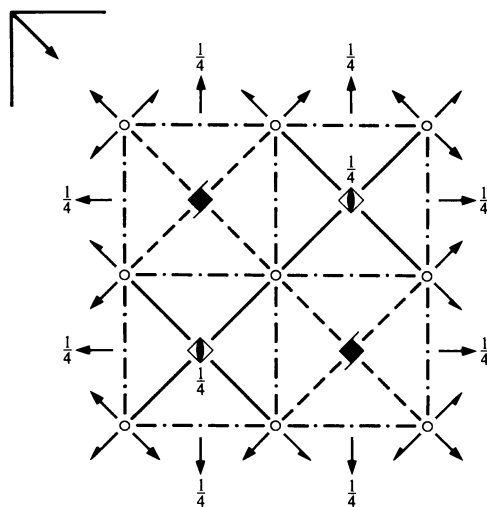
$P4_2/nnm$ D_{4h}^{12} $4/mmm$

Tetragonal

No. 134

 $P 4_2/n 2/n 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2

Origin at centre ($2/m$) at $nn(2_1/g, 2/m)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}2m$ Asymmetric unit $-\frac{1}{4} \leq x \leq \frac{1}{4}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}; x \leq -y$

Symmetry operations

- | | | | |
|-----------------------------------------------|-----------------------------------------------|---------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| (1) 1 | (2) $2 \frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ | (4) $4^-(0, 0, \frac{1}{2}) \frac{1}{4}, \frac{1}{4}, z$ |
| (5) $2 \frac{1}{4}, y, \frac{1}{4}$ | (6) $2 x, \frac{1}{4}, \frac{1}{4}$ | (7) $2 x, x, 0$ | (8) $2 x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1} 0, 0, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, 0$ | (11) $\bar{4}^+ \frac{1}{4}, -\frac{1}{4}, z; \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ | (12) $\bar{4}^- -\frac{1}{4}, \frac{1}{4}, z; -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2}) x, 0, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2}) 0, y, z$ | (15) $m x, \bar{x}, z$ | (16) $g(\frac{1}{2}, \frac{1}{2}, 0) x, x, z$ |

Maximal non-isomorphic subgroups

- I** [2] $P\bar{4}n2$ (118) 1; 2; 7; 8; 11; 12; 13; 14
 [2] $P\bar{4}2m$ (111) 1; 2; 5; 6; 11; 12; 15; 16
 [2] $P4_2nm$ (102) 1; 2; 3; 4; 13; 14; 15; 16
 [2] $P4_222$ (93) 1; 2; 3; 4; 5; 6; 7; 8
 [2] $P4_2/n11$ ($P4_2/n$, 86) 1; 2; 3; 4; 9; 10; 11; 12
 [2] $P2/n12/m$ ($Cmme$, 67) 1; 2; 7; 8; 9; 10; 15; 16
 [2] $P2/n2/n1$ ($Pnmm$, 48) 1; 2; 5; 6; 9; 10; 13; 14

IIa none**IIb** [2] $F4_1/ddc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/acd$, 142); [2] $F4_1/ddm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4_1/amd$, 141)**Maximal isomorphic subgroups of lowest index****IIc** [3] $P4_2/nnm$ ($\mathbf{c}' = 3\mathbf{c}$) (134); [9] $P4_2/nnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (134)**Minimal non-isomorphic supergroups****I** [3] $Pn\bar{3}m$ (224)**II** [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>n</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z + \frac{1}{2}$ (4) $y, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
8 <i>m</i> $\dots m$	x, \bar{x}, z $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x + \frac{1}{2}, x, z + \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$ $x, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ \bar{x}, x, \bar{z} $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>l</i> $\dots 2$	$x, x, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, 0$ $x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, \bar{x}, \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	$hkl : h + k = 2n$
8 <i>k</i> $\dots 2$	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
8 <i>j</i> $\dots 2$	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$	$hkl : h + k + l = 2n$
8 <i>i</i> $\dots 2$	$x, \frac{1}{4}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>h</i> $2 \dots$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, z$	$hkl : h + k, l = 2n$
4 <i>g</i> $2 \dots mm$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	$hkl : h + k + l = 2n$
4 <i>f</i> $\dots 2/m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ $0, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>e</i> $\dots 2/m$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$
4 <i>d</i> $2 \dots 22$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> $222 \dots$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>b</i> $\bar{4}2m$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}2m$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along $[001]$ $p4mm$

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

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

Along $[100]$ $c2mm$

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

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

Along $[110]$ $p2mm$

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

Origin at $x, x, 0$

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