

$P4/nnc$

D_{4h}^4

$4/mmm$

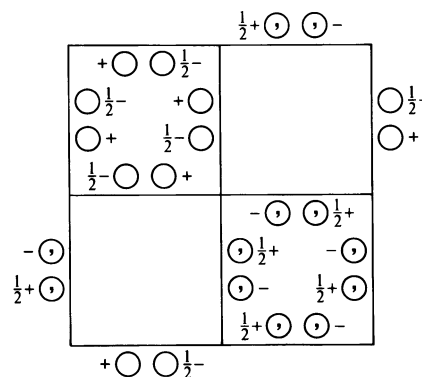
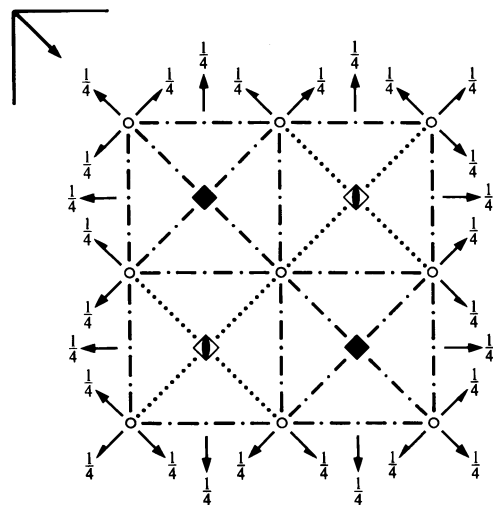
Tetragonal

No. 126

$P 4/n 2/n 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $nn(n,c)$, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from 422

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

Symmetry operations

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

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>k</i> 1	(1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{y} + \frac{1}{2}, x, z$ (4) $y, \bar{x} + \frac{1}{2}, z$ (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) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (12) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $hk0 : h + k = 2n$ $0kl : k + l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
8 <i>j</i> .2.	$x, \frac{3}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>i</i> .2.	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{1}{4}$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>h</i> ..2	$x, x, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>g</i> 2..	$\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>f</i> $\bar{1}$	0,0,0 $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ 0, $\frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$ 0, $\frac{1}{2}, \frac{1}{2}$ 0, 0, $\frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k, l = 2n$
4 <i>e</i> 4..	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4}$..	$\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>c</i> 222.	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k, l = 2n$
2 <i>b</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> 422	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4mm$

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

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] $p2mm$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/c$ ($Ccce$, 68)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/n1$ ($Pnnn$, 48)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/nnc$ ($c' = 3c$) (126); [9] $P4/nnc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (126)

Minimal non-isomorphic supergroups

I [3] $Pn\bar{3}n$ (222)

II [2] $I4/mmm$ (139); [2] $C4/mcc$ ($P4/mcc$, 124); [2] $P4/nbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (125)