

$P4/ncc$

D_{4h}^8

$4/mmm$

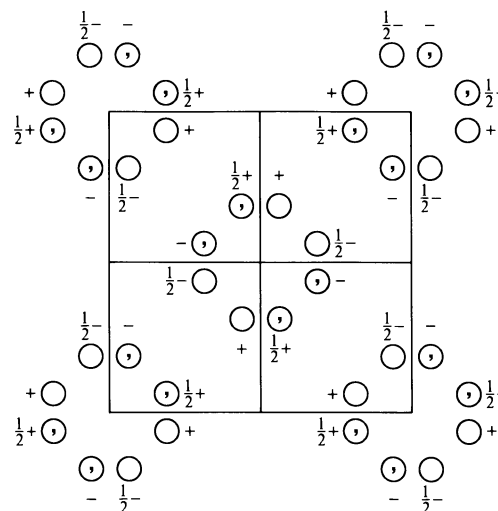
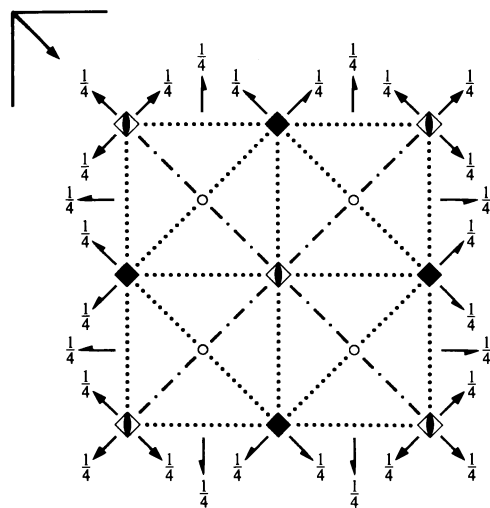
Tetragonal

No. 130

$P 4/n 2_1/c 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}/ncn$, at $-\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

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

Symmetry operations

- | | | | |
|--|--|--|---|
| (1) 1 | (2) 2 $0, 0, z$ | (3) 4^+ $0, \frac{1}{2}, z$ | (4) 4^- $-\frac{1}{2}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $\frac{1}{4}, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, \frac{1}{4}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ | (11) $\bar{4}^+$ $0, 0, z; 0, 0, 0$ | (12) $\bar{4}^-$ $0, 0, z; 0, 0, 0$ |
| (13) c $x, 0, z$ | (14) c $0, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (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
		General:
16 <i>g</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \bar{z} (13) $x, \bar{y}, z + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	$hk0 : h + k = 2n$ $0kl : l = 2n$ $hhl : l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>f</i> ..2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x, \bar{x}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl : h + k + l = 2n$
8 <i>e</i> 2..	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$ $0, 0, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k, l = 2n$
8 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$hkl : h, k, l = 2n$
4 <i>c</i> 4..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$hkl : h + k, l = 2n$
4 <i>a</i> 2.22	$0, 0, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$ $0, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$

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 $0, 0, z$

Along [100] $p2mg$

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

Origin at $x, \frac{1}{4}, 0$

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] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22$ (90)	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] $P2/n2_1/c1$ ($Pccn$, 56)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4/ncc$ ($\mathbf{c}' = 3\mathbf{c}$) (130); [9] $P4/ncc$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (130)

Minimal non-isomorphic supergroups

I none

II [2] $C4/mcc$ ($P4/mcc$, 124); [2] $I4/mcm$ (140); [2] $P4/nmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (129)