

$P\bar{4}c2$

D_{2d}^6

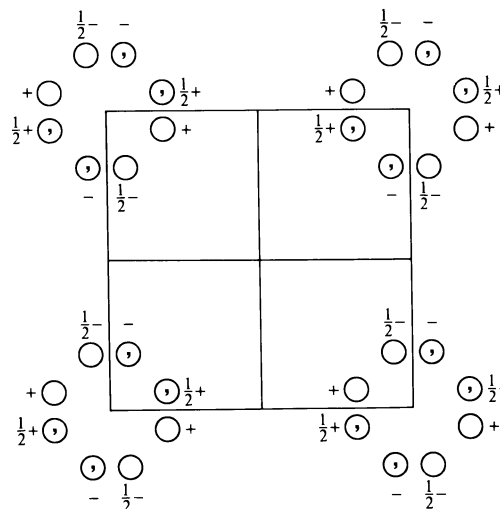
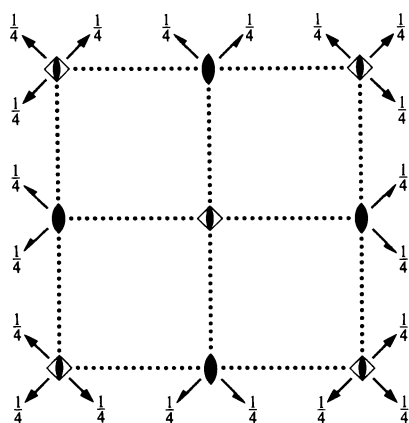
$\bar{4}m2$

Tetragonal

No. 116

$P\bar{4}c2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}c1$

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

Symmetry operations

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

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

Positions

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

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

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

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
 [2] $P2c1$ ($Pcc2$, 27) 1; 2; 5; 6
 [2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $C\bar{4}c2_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2_1c$, 114); [2] $C\bar{4}c2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}2c$, 112)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}c2$ ($\mathbf{c}' = 3\mathbf{c}$) (116); [9] $P\bar{4}c2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (116)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/ncc$ (130); [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)
II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}c2$ (120); [2] $P\bar{4}m2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (115)