

$P\bar{4}b2$

D_{2d}^7

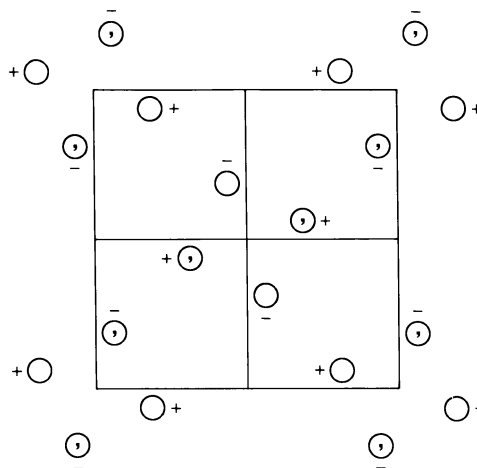
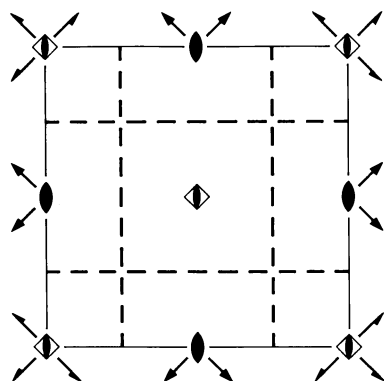
$\bar{4}m2$

Tetragonal

No. 117

$P\bar{4}b2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}12_1$

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

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) a $x, \frac{1}{4}, z$ | (6) b $\frac{1}{4}, y, z$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) x, x, 0$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |

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>i</i> 1	(1) x, y, z (5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$
	(3) y, \bar{x}, \bar{z} (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(4) \bar{y}, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$
		General: $Ok\ell : k = 2n$ $h00 : h = 2n$
		Special: as above, plus
4 <i>h</i> ..2	$x, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, \frac{1}{2}$	no extra conditions
4 <i>g</i> ..2	$x, x + \frac{1}{2}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x, 0$	no extra conditions
4 <i>f</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$	$hkl : h + k = 2n$
4 <i>e</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$	$hkl : h + k = 2n$
2 <i>d</i> 2.22	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>c</i> 2.22	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hkl : h + k = 2n$
2 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k = 2n$
2 <i>a</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

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

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
 [2] $P2b1$ ($Pba2$, 32) 1; 2; 5; 6
 [2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIb [2] $P\bar{4}n2$ ($\mathbf{c}' = 2\mathbf{c}$) (118)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}b2$ ($\mathbf{c}' = 2\mathbf{c}$) (117); [9] $P\bar{4}b2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (117)

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4/mbm$ (127); [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

II [2] $C\bar{4}m2$ ($P\bar{4}2m$, 111); [2] $I\bar{4}c2$ (120)