

$P\bar{4}n2$

D_{2d}^8

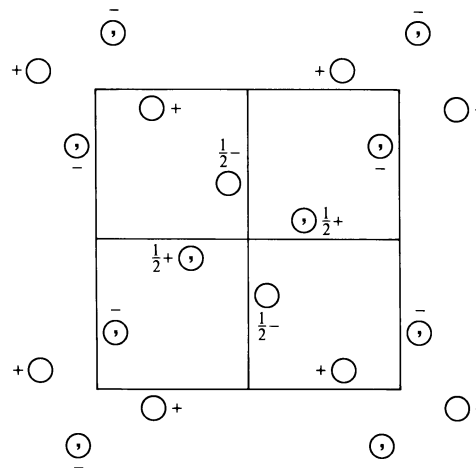
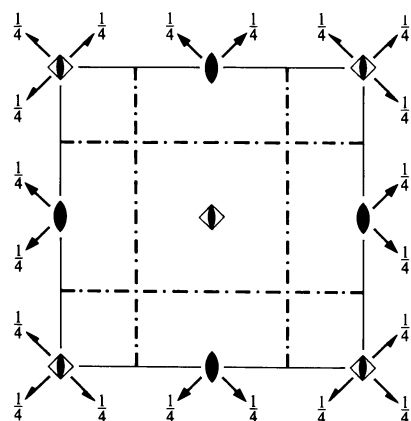
$\bar{4}m2$

Tetragonal

No. 118

$P\bar{4}n2$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}$

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

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 (2) \bar{x}, \bar{y}, z (3) y, \bar{x}, \bar{z} (4) \bar{y}, x, \bar{z} (5) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	General: $0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$ Special: as above, plus
4 <i>h</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>g</i> ..2	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>f</i> ..2	$x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, \bar{x}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>e</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>d</i> 2..22	$0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$	$hkl : h + k + l = 2n$
2 <i>c</i> 2..22	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>b</i> $\bar{4}$..	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> $\bar{4}$..	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

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

Along $[100]$ $c1m1$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

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

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P2n1$ ($Pnn2$, 34) 1; 2; 5; 6
[2] $P212$ ($C222$, 21) 1; 2; 7; 8

IIa none

IIIb [2] $F\bar{4}d2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}2d$, 122)

Maximal isomorphic subgroups of lowest index

IIIc [3] $P\bar{4}n2$ ($\mathbf{c}' = 3\mathbf{c}$) (118); [9] $P\bar{4}n2$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (118)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/mnc$ (128); [2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II [2] $C\bar{4}c2$ ($P\bar{4}2c$, 112); [2] $I\bar{4}m2$ (119); [2] $P\bar{4}b2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (117)