

$P\bar{4}2m$

D_{2d}^1

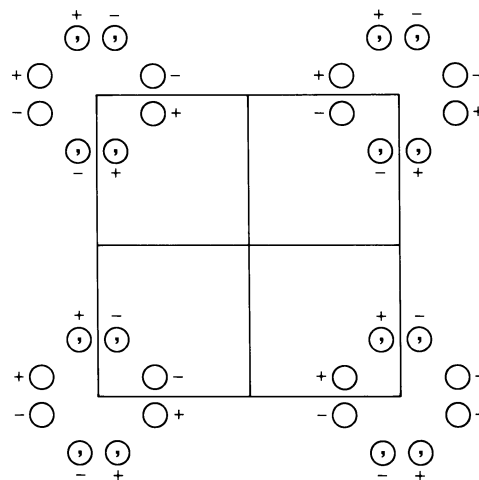
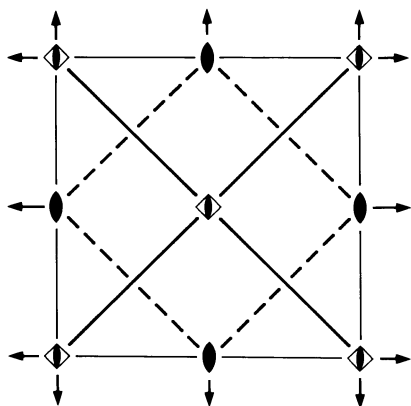
$\bar{4}2m$

Tetragonal

No. 111

$P\bar{4}2m$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}2m$

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

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) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) m x,\bar{x},z | (8) m x,x,z |

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

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p1m1$

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

Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}11$ ($P\bar{4}$, 81)	1; 2; 3; 4
	[2] $P21m$ ($Cmm2$, 35)	1; 2; 7; 8
	[2] $P221$ ($P222$, 16)	1; 2; 5; 6

IIa none

IIb [2] $P\bar{4}2c$ ($\mathbf{c}' = 2\mathbf{c}$) (112); [2] $C\bar{4}2d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}b2$, 117); [2] $C\bar{4}2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}m2$, 115); [2] $F\bar{4}2c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}c2$, 120); [2] $F\bar{4}2m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I\bar{4}m2$, 119)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}2m$ ($\mathbf{c}' = 2\mathbf{c}$) (111); [9] $P\bar{4}2m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (111)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nbm$ (125); [2] $P4_2/mcm$ (132); [2] $P4_2/nnm$ (134); [3] $P\bar{4}3m$ (215)

II [2] $C\bar{4}2m$ ($P\bar{4}m2$, 115); [2] $I\bar{4}2m$ (121)