

$P\bar{4}2c$

D_{2d}^2

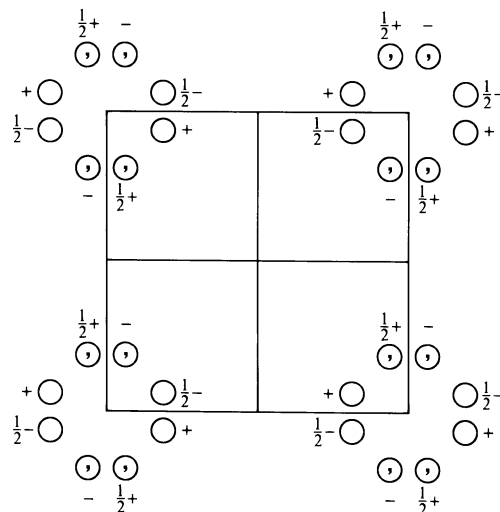
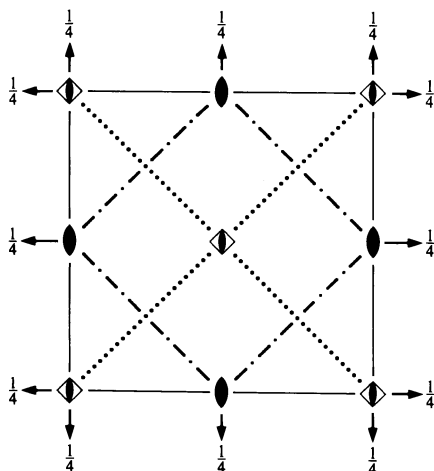
$\bar{4}2m$

Tetragonal

No. 112

$P\bar{4}2c$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1c$

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) 2 $0, y, \frac{1}{4}$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) c x, \bar{x}, z | (8) c 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>n</i> 1	(1) x, y, z (5) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (2) \bar{x}, \bar{y}, z (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (3) y, \bar{x}, \bar{z} (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (4) \bar{y}, x, \bar{z} (8) $y, x, z + \frac{1}{2}$	General: $hkl : l = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>m</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>l</i> 2..	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>k</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$ $0, 0, z + \frac{1}{2}$	$hkl : l = 2n$
4 <i>j</i> .2.	$0, y, \frac{1}{4}$ $0, \bar{y}, \frac{1}{4}$ $y, 0, \frac{3}{4}$ $\bar{y}, 0, \frac{3}{4}$	no extra conditions
4 <i>i</i> .2.	$x, \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \bar{x}, \frac{3}{4}$ $\frac{1}{2}, x, \frac{3}{4}$	no extra conditions
4 <i>h</i> .2.	$\frac{1}{2}, y, \frac{1}{4}$ $\frac{1}{2}, \bar{y}, \frac{1}{4}$ $y, \frac{1}{2}, \frac{3}{4}$ $\bar{y}, \frac{1}{2}, \frac{3}{4}$	no extra conditions
4 <i>g</i> .2.	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{1}{4}$ $0, \bar{x}, \frac{3}{4}$ $0, x, \frac{3}{4}$	no extra conditions
2 <i>f</i> $\bar{4}$..	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
2 <i>e</i> $\bar{4}$..	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : l = 2n$
2 <i>d</i> 222.	$0, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>c</i> 222.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
2 <i>b</i> 222.	$\frac{1}{2}, 0, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$
2 <i>a</i> 222.	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkl : l = 2n$

Symmetry of special projections

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

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, \frac{1}{4}$

Along [110] $p1m1$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P\bar{4}11$ ($P\bar{4}$, 81) 1; 2; 3; 4
[2] $P21c$ ($Ccc2$, 37) 1; 2; 7; 8
[2] $P221$ ($P222$, 16) 1; 2; 5; 6

IIa none

IIb [2] $C\bar{4}2d$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}n2$, 118); [2] $C\bar{4}2c$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P\bar{4}c2$, 116)

Maximal isomorphic subgroups of lowest index

IIc [3] $P\bar{4}2c$ ($\mathbf{c}' = 3\mathbf{c}$) (112); [9] $P\bar{4}2c$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (112)

Minimal non-isomorphic supergroups

I [2] $P4/mcc$ (124); [2] $P4/nnc$ (126); [2] $P4_2/mmc$ (131); [2] $P4_2/nbc$ (133); [3] $P\bar{4}3n$ (218)

II [2] $C\bar{4}2c$ ($P\bar{4}c2$, 116); [2] $I\bar{4}2m$ (121); [2] $P\bar{4}2m$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (111)