

$P\bar{4}2_1m$

D_{2d}^3

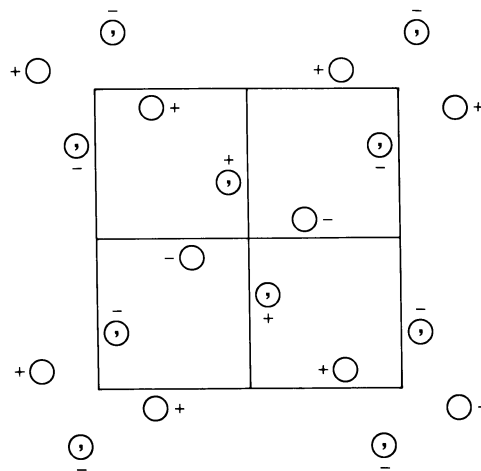
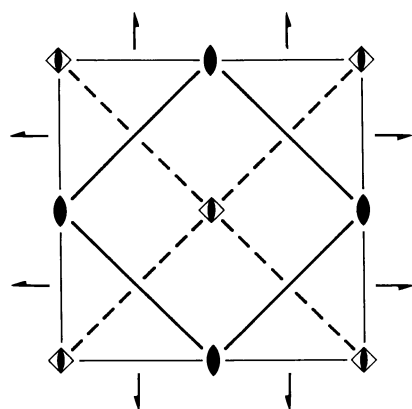
$\bar{4}2m$

Tetragonal

No. 113

$P\bar{4}2_1m$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1g$

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

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

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>f</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(3) y, \bar{x}, \bar{z} (7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) \bar{y}, x, \bar{z} (8) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk0 : h = 2n$ Special: as above, plus no extra conditions
4 <i>e</i> $\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, \bar{z}$	$hkl : h + k = 2n$
4 <i>d</i> $2 \dots$	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hk0 : h + k = 2n$
2 <i>c</i> $2 \dots mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			$hkl : h + k = 2n$
2 <i>b</i> $\bar{4} \dots$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : h + k = 2n$
2 <i>a</i> $\bar{4} \dots$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl : h + k = 2n$

Symmetry of special projections

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

Along $[100]$ $p2mg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, 0$

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] $P22_11$ ($P2_12_12$, 18) 1; 2; 5; 6

IIa none

IIb [2] $P\bar{4}2_1c$ ($c' = 2c$) (114)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{4}2_1m$ ($c' = 2c$) (113); [9] $P\bar{4}2_1m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (113)

Minimal non-isomorphic supergroups

I [2] $P4/mbm$ (127); [2] $P4/nmm$ (129); [2] $P4_2/mnm$ (136); [2] $P4_2/ncm$ (138)

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