

$P\bar{4}2_1c$

D_{2d}^4

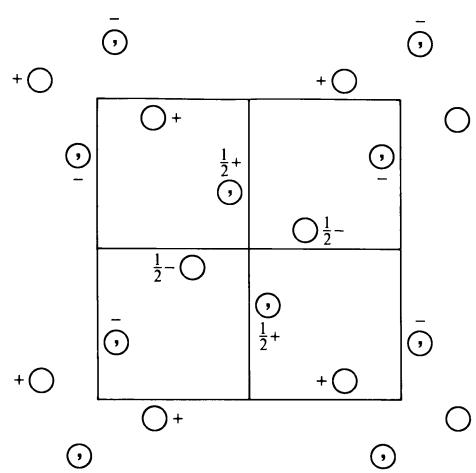
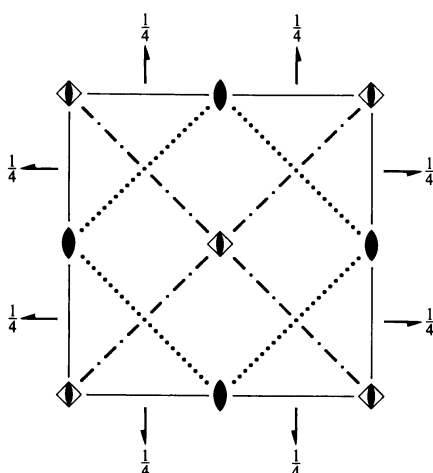
$\bar{4}2m$

Tetragonal

No. 114

$P\bar{4}2_1c$

Patterson symmetry $P4/mmm$



Origin at $\bar{4}1n$

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

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>e</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) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (8) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$	General: $hkl: l = 2n$ $00l: l = 2n$ $h00: h = 2n$
4 <i>d</i> 2..	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, \bar{z}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $0, \frac{1}{2}, z + \frac{1}{2}$	Special: as above, plus $hkl: l = 2n$ $hk0: h + k = 2n$
4 <i>c</i> 2..	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
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 $[001] \ p4gm$
 $\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

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

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