

$P\bar{4}n2$

$D_{2d}^8$

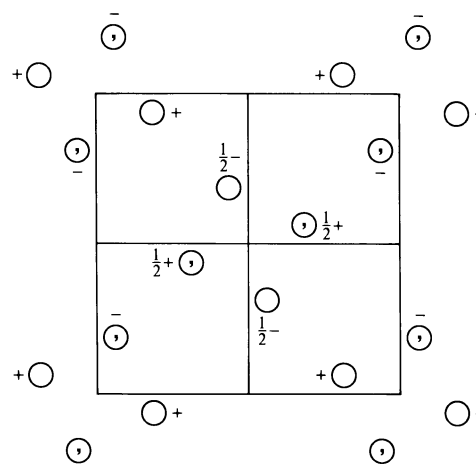
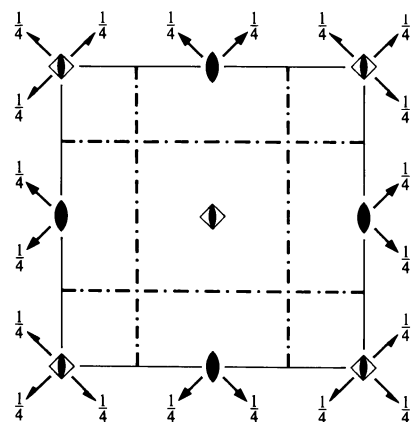
$\bar{4}m2$

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: $Ok\bar{l}: k+l=2n$ $00l: l=2n$ $h00: h=2n$ 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  $x,x,\frac{1}{4}$