

$P\bar{4}c2$

$D_{2d}^6$

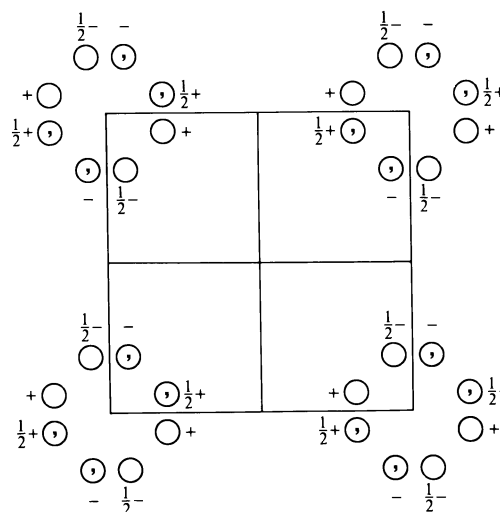
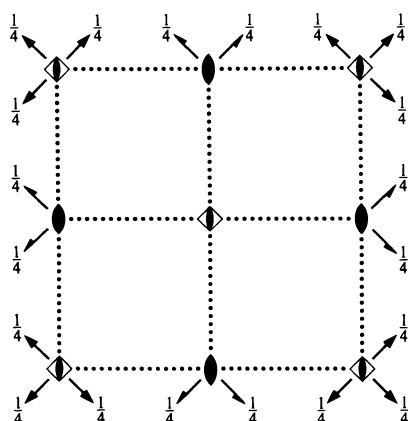
$\bar{4}m2$

Tetragonal

No. 116

$P\bar{4}c2$

Patterson symmetry  $P4/mmm$



Origin at  $\bar{4}c1$

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

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>j</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) $x,\bar{y},z+\frac{1}{2}$ (6) $\bar{x},y,z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	General: $0kl: l = 2n$ $00l: l = 2n$
4 <i>i</i> 2..	$0,\frac{1}{2},z$ $\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$	Special: as above, plus $hkl: l = 2n$ $hk0: h+k = 2n$
4 <i>h</i> 2..	$\frac{1}{2},\frac{1}{2},z$ $\frac{1}{2},\frac{1}{2},\bar{z}$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl: l = 2n$
4 <i>g</i> 2..	$0,0,z$ $0,0,\bar{z}$ $0,0,z+\frac{1}{2}$ $0,0,\bar{z}+\frac{1}{2}$	$hkl: l = 2n$
4 <i>f</i> ..2	$x,x,\frac{3}{4}$ $\bar{x},\bar{x},\frac{3}{4}$ $x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{1}{4}$	no extra conditions
4 <i>e</i> ..2	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$ $\bar{x},x,\frac{3}{4}$	no extra conditions
2 <i>d</i> $\bar{4}$ ..	$\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkl: l = 2n$
2 <i>c</i> $\bar{4}$ ..	$0,0,0$ $0,0,\frac{1}{2}$	$hkl: l = 2n$
2 <i>b</i> 2..22	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$hkl: l = 2n$
2 <i>a</i> 2..22	$0,0,\frac{1}{4}$ $0,0,\frac{3}{4}$	$hkl: l = 2n$

Symmetry of special projections

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

Along  $[100]$   $p1m1$   
 $\mathbf{a}' = \mathbf{b}$   $\mathbf{b}' = \frac{1}{2}\mathbf{c}$   
 Origin at  $x,0,0$

Along  $[110]$   $p2mm$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$   $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x,x,\frac{1}{4}$