

$P4/mmm$

D_{4h}^1

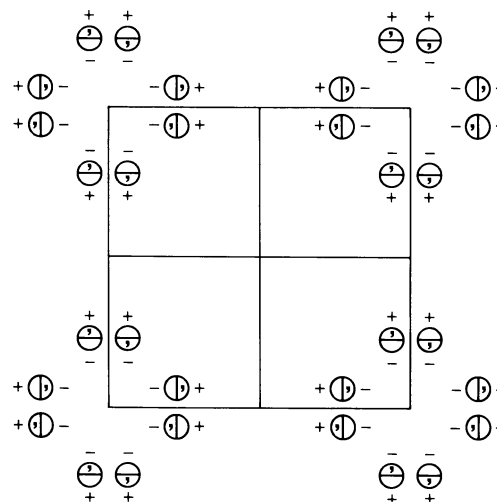
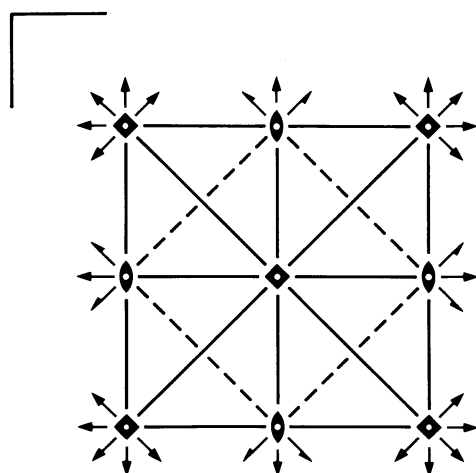
$4/mmm$

Tetragonal

No. 123

$P 4/m 2/m 2/m$

Patterson symmetry $P4/mmm$



Origin at centre ($4/mmm$)

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

Symmetry operations

- | | | | |
|-----------------------|------------------|---------------------------------|---------------------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,0$ | (8) 2 $x,\bar{x},0$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (13) m $x,0,z$ | (14) m $0,y,z$ | (15) m x,\bar{x},z | (16) m x,x,z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
16	<i>u</i> 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	no conditions
8	<i>t</i> . <i>m</i> .	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	no extra conditions
8	<i>s</i> . <i>m</i> .	$x, 0, z$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z$ $x, 0, \bar{z}$	$0, x, z$ $0, x, \bar{z}$	$0, \bar{x}, z$ $0, \bar{x}, \bar{z}$	no extra conditions
8	<i>r</i> . . <i>m</i>	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	\bar{x}, x, z x, x, \bar{z}	x, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8	<i>q</i> <i>m</i> . .	$x, y, \frac{1}{2}$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	<i>p</i> <i>m</i> . .	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
4	<i>o</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>n</i> <i>m</i> 2 <i>m</i> .	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	<i>m</i> <i>m</i> 2 <i>m</i> .	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>l</i> <i>m</i> 2 <i>m</i> .	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	<i>k</i> <i>m</i> . 2 <i>m</i>	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>j</i> <i>m</i> . 2 <i>m</i>	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4	<i>i</i> 2 <i>m</i> <i>m</i> .	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl: h+k=2n$
2	<i>h</i> 4 <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2	<i>g</i> 4 <i>m</i> <i>m</i>	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2	<i>f</i> <i>m</i> <i>m</i> <i>m</i> .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl: h+k=2n$
2	<i>e</i> <i>m</i> <i>m</i> <i>m</i> .	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h+k=2n$
1	<i>d</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1	<i>c</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1	<i>b</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, \frac{1}{2}$				no extra conditions
1	<i>a</i> 4/ <i>m</i> <i>m</i> <i>m</i>	$0, 0, 0$				no extra conditions

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 $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$