

$P4_2/mmc$

D_{4h}^9

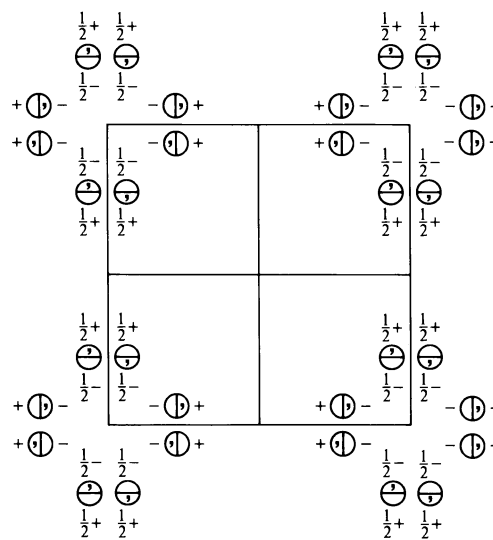
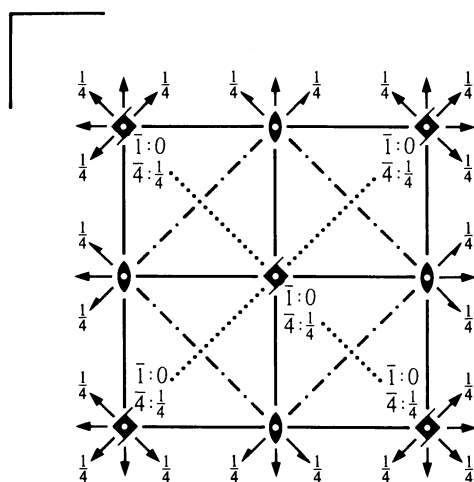
$4/mmm$

Tetragonal

No. 131

$P 4_2/m 2/m 2/c$

Patterson symmetry $P4/mmm$



Origin at centre (mmm) at $4_2/m2/mc$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | | |
|-----------------------|------------------|--|--|
| (1) 1 | (2) 2 $0,0,z$ | (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$ |
| (5) 2 $0,y,0$ | (6) 2 $x,0,0$ | (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,\bar{x},\frac{1}{4}$ |
| (9) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z$; $0,0,\frac{1}{4}$ | (12) $\bar{4}^-$ $0,0,z$; $0,0,\frac{1}{4}$ |
| (13) m $x,0,z$ | (14) m $0,y,z$ | (15) c x,\bar{x},z | (16) c 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>r</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) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	$hhl: l = 2n$ $00l: l = 2n$
Special: as above, plus						
8	<i>q</i> $m..$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	<i>p</i> $.m.$	$\frac{1}{2}, y, z$ $\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, z$ $\frac{1}{2}, \bar{y}, \bar{z}$	$\bar{y}, \frac{1}{2}, z + \frac{1}{2}$ $y, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$y, \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	<i>o</i> $.m.$	$0, y, z$ $0, y, \bar{z}$	$0, \bar{y}, z$ $0, \bar{y}, \bar{z}$	$\bar{y}, 0, z + \frac{1}{2}$ $y, 0, \bar{z} + \frac{1}{2}$	$y, 0, z + \frac{1}{2}$ $\bar{y}, 0, \bar{z} + \frac{1}{2}$	no extra conditions
8	<i>n</i> $..2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$ $x, x, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$ $x, \bar{x}, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$ $\bar{x}, x, \frac{3}{4}$	$hkl: l = 2n$
4	<i>m</i> $m2m.$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>l</i> $m2m.$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	<i>k</i> $m2m.$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	<i>j</i> $m2m.$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	<i>i</i> $2mm.$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl: h + k + l = 2n$
4	<i>h</i> $2mm.$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl: l = 2n$
4	<i>g</i> $2mm.$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl: l = 2n$
2	<i>f</i> $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl: l = 2n$
2	<i>e</i> $\bar{4}m2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl: l = 2n$
2	<i>d</i> $mmm.$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl: h + k + l = 2n$
2	<i>c</i> $mmm.$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + k + l = 2n$
2	<i>b</i> $mmm.$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: l = 2n$
2	<i>a</i> $mmm.$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl: l = 2n$

Symmetry of special projections

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

Along [100] $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

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