

$I4/mmm$

D_{4h}^{17}

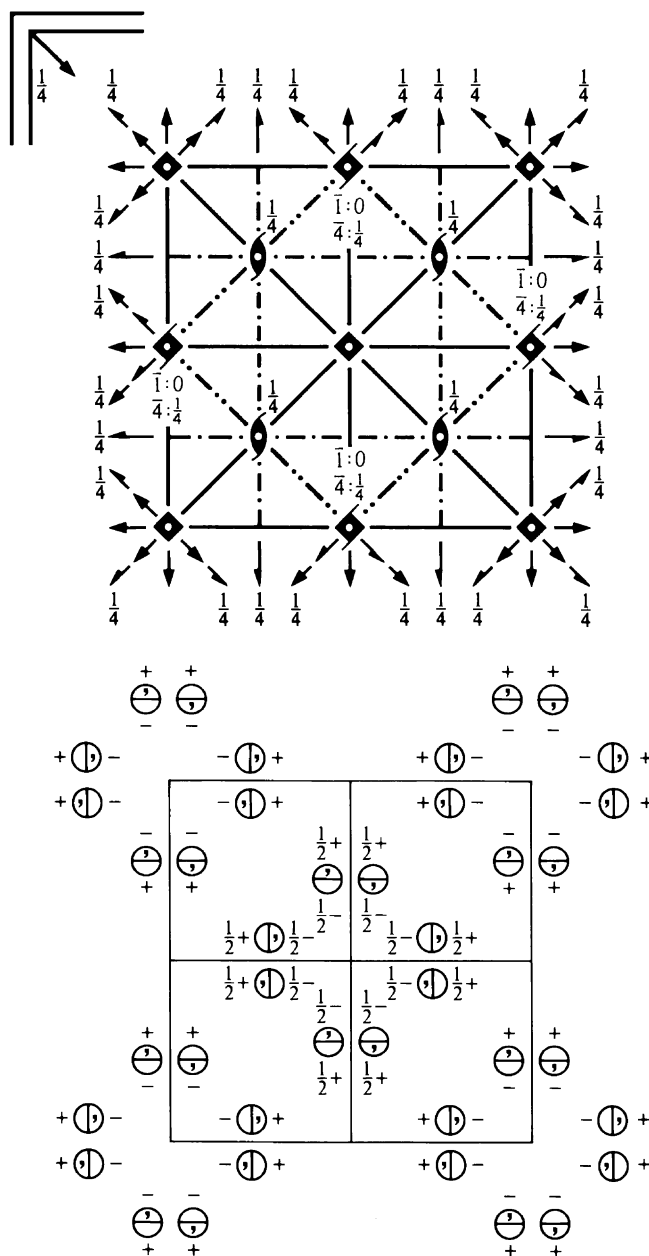
$4/mmm$

Tetragonal

No. 139

$I 4/m 2/m 2/m$

Patterson symmetry $I4/mmm$



Origin at centre ($4/mmm$)

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

Symmetry operations

For $(0,0,0)+$ set

- | | | | |
|-----------------------|------------------|---------------------------|---------------------------|
| (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) 4^+ $0,0,z; 0,0,0$ | (12) 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 |

For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set

- | | | | |
|---|---|---|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (2) $2(0,0, \frac{1}{2})$ $\frac{1}{4}, \frac{1}{4}, z$ | (3) $4^+(0,0, \frac{1}{2})$ $0, \frac{1}{2}, z$ | (4) $4^-(0,0, \frac{1}{2})$ $\frac{1}{2}, 0, z$ |
| (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) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, \frac{1}{4}$ | (11) 4^+ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (12) 4^- $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |
| (13) $n(\frac{1}{2}, 0, \frac{1}{2})$ $x, \frac{1}{4}, z$ | (14) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{4}, y, z$ | (15) c $x + \frac{1}{2}, \bar{x}, z$ | (16) $n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, z |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$				Reflection conditions
32 <i>o</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	General: $hkl: h+k+l=2n$ $hk0: h+k=2n$ $0kl: k+l=2n$ $hhl: l=2n$ $00l: l=2n$ $h00: h=2n$ Special: as above, plus
16 <i>n</i> $.m.$	$0, y, z$ $0, y, \bar{z}$	$0, \bar{y}, z$ $0, \bar{y}, \bar{z}$	$\bar{y}, 0, z$ $y, 0, \bar{z}$	$y, 0, z$ $\bar{y}, 0, \bar{z}$	no extra conditions
16 <i>m</i> $.m$	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
16 <i>l</i> $m..$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
16 <i>k</i> $..2$	$x, x + \frac{1}{2}, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, \frac{3}{4}$	$\bar{x}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x, x + \frac{1}{2}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, x, \frac{1}{4}$ $x + \frac{1}{2}, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, \frac{1}{4}$ $\bar{x} + \frac{1}{2}, x, \frac{3}{4}$	$hkl: l=2n$
8 <i>j</i> $m2m.$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
8 <i>i</i> $m2m.$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
8 <i>h</i> $m.2m$	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
8 <i>g</i> $2mm.$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl: l=2n$
8 <i>f</i> $..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl: k, l=2n$
4 <i>e</i> $4mm$	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4 <i>d</i> $\bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$			$hkl: l=2n$
4 <i>c</i> $mmm.$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl: l=2n$
2 <i>b</i> $4/mmm$	$0, 0, \frac{1}{2}$				no extra conditions
2 <i>a</i> $4/mmm$	$0, 0, 0$				no extra conditions

Symmetry of special projectionsAlong [001] $p4mm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at $0, 0, z$ Along [100] $c2mm$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at $x, 0, 0$ Along [110] $p2mm$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at $x, x, 0$