

$I4/mcm$

D_{4h}^{18}

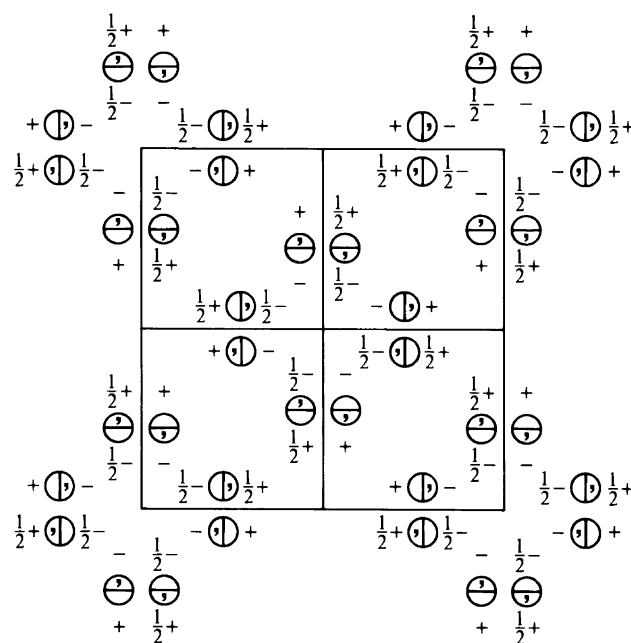
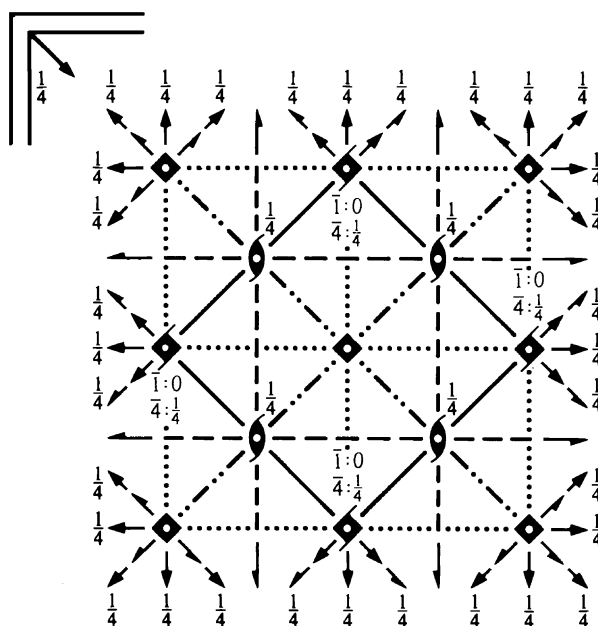
$4/mmm$

Tetragonal

No. 140

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

Patterson symmetry $I4/mmm$



Origin at centre ($4/m$) at $4/mc2_1/e$

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

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 $0,y,\frac{1}{4}$ | (6) 2 $x,0,\frac{1}{4}$ | (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) $\bar{4}^+$ $0,0,z$; $0,0,0$ | (12) $\bar{4}^-$ $0,0,z$; $0,0,0$ |
| (13) c $x,0,z$ | (14) c $0,y,z$ | (15) c x,\bar{x},z | (16) c 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 $(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ | (6) 2 $(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ | (7) 2 $(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$ | (8) 2 $x,\bar{x}+\frac{1}{2},0$ |
| (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) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$ | (12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$ |
| (13) a $x,\frac{1}{4},z$ | (14) b $\frac{1}{4},y,z$ | (15) m $x+\frac{1}{2},\bar{x},z$ | (16) $g(\frac{1}{2},\frac{1}{2},0)$ 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

General:

32	<i>m</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z
			(5) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) x, y, \bar{z}	(11) y, \bar{x}, \bar{z}	(12) \bar{y}, x, \bar{z}
			(13) $x, \bar{y}, z + \frac{1}{2}$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(16) $y, x, z + \frac{1}{2}$

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>l</i>	$\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$\bar{x} + \frac{1}{2}, x, z$	$x + \frac{1}{2}, \bar{x}, z$
			$\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$

no extra conditions

16	<i>k</i>	$m \dots$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, 0$	$y, \bar{x}, 0$
			$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$	$y, x, \frac{1}{2}$	$\bar{y}, \bar{x}, \frac{1}{2}$

no extra conditions

16	<i>j</i>	$.2.$	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$0, \bar{x}, \frac{1}{4}$
			$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$0, x, \frac{3}{4}$

hkl : $l = 2n$

16	<i>i</i>	$\dots 2$	$x, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$
			$\bar{x}, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	$x, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$

hkl : $l = 2n$

8	<i>h</i>	$m . 2m$	$x, x + \frac{1}{2}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, 0$	$x + \frac{1}{2}, \bar{x}, 0$
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no extra conditions

8	<i>g</i>	$2 . mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$
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hkl : $l = 2n$

8	<i>f</i>	$4 \dots$	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$
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hkl : $l = 2n$

8	<i>e</i>	$\dots 2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$
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hkl : $k, l = 2n$

4	<i>d</i>	$m . mm$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$
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hkl : $l = 2n$

4	<i>c</i>	$4/m \dots$	$0, 0, 0$	$0, 0, \frac{1}{2}$
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hkl : $l = 2n$

4	<i>b</i>	$\bar{4} 2 m$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$
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hkl : $l = 2n$

4	<i>a</i>	$4 2 2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$
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hkl : $l = 2n$

Symmetry of special projections

Along [001] $p4mm$

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

Origin at $0, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [110] $p2mm$

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

Origin at $x, x, 0$