

$I4/m$

$C_{4h}^5$

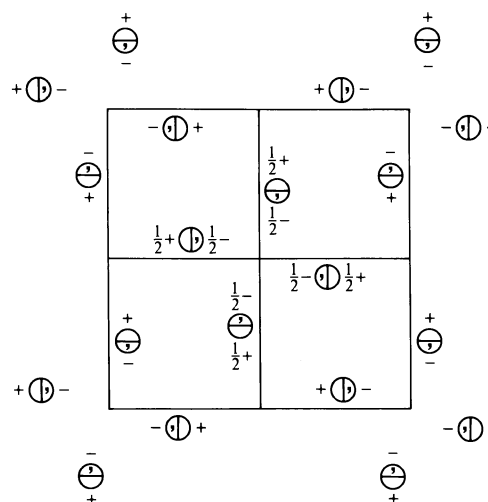
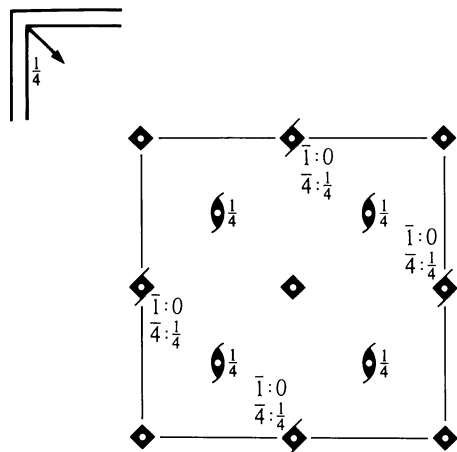
$4/m$

Tetragonal

No. 87

$I4/m$

Patterson symmetry  $I4/m$



**Origin** at centre ( $4/m$ )

**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**

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

- |                     |                       |                              |                              |
|---------------------|-----------------------|------------------------------|------------------------------|
| (1) 1               | (2) $2 \bar{1} 0,0,z$ | (3) $4^+ 0,0,z$              | (4) $4^- 0,0,z$              |
| (5) $\bar{1} 0,0,0$ | (6) $m x,y,0$         | (7) $\bar{4}^+ 0,0,z; 0,0,0$ | (8) $\bar{4}^- 0,0,z; 0,0,0$ |

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

- |   |  |  |  |
|---|--|--|--|
| (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$      | (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) $\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) x, y, \frac{1}{4}$ | (7) $\bar{4}^+ \frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$ | (8) $\bar{4}^- 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ |

**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)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
		$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:
16	<i>i</i> 1	(1) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x}, \bar{y}, z$ (6) $x, y, \bar{z}$	(3) $\bar{y}, x, z$ (7) $y, \bar{x}, \bar{z}$	(4) $y, \bar{x}, z$ (8) $\bar{y}, x, \bar{z}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=2n$ $h00 : h=2n$
8	<i>h</i> $m..$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, 0$	$y, \bar{x}, 0$	Special: as above, plus no extra conditions
8	<i>g</i> $2..$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl : l=2n$
8	<i>f</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : k, l=2n$
4	<i>e</i> $4..$	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
4	<i>d</i> $\bar{4}..$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$			$hkl : l=2n$
4	<i>c</i> $2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl : l=2n$
2	<i>b</i> $4/m..$	$0, 0, \frac{1}{2}$				no extra conditions
2	<i>a</i> $4/m..$	$0, 0, 0$				no extra conditions

**Symmetry of special projections**

Along [001]  $p4$

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

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  $x, x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+
	[2] $I4$ (79)	(1; 2; 3; 4)+
	[2] $I2/m$ ( $C2/m$ , 12)	(1; 2; 5; 6)+
<b>IIa</b>	[2] $P4_2/n$ (86)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4/n$ (85)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4_2/m$ (84)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $P4/m$ (83)	1; 2; 3; 4; 5; 6; 7; 8
<b>IIb</b>	none	

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $I4/m$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (87); [5]  $I4/m$  ( $\mathbf{a}' = \mathbf{a} + 2\mathbf{b}, \mathbf{b}' = -2\mathbf{a} + \mathbf{b}$  or  $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}, \mathbf{b}' = 2\mathbf{a} + \mathbf{b}$ ) (87)

**Minimal non-isomorphic supergroups**

<b>I</b>	[2] $I4/mmm$ (139); [2] $I4/mcm$ (140)
<b>II</b>	[2] $C4/m$ ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P4/m$ , 83)