

*Pccm*

$D_{2h}^3$

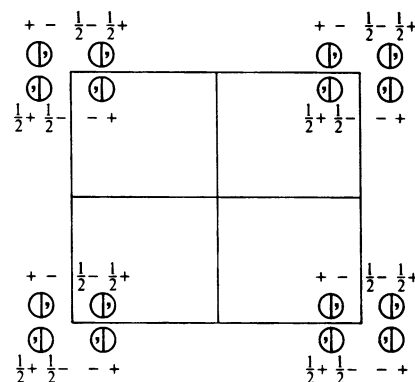
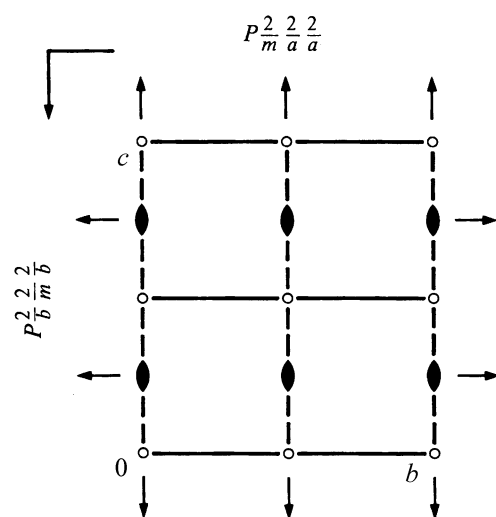
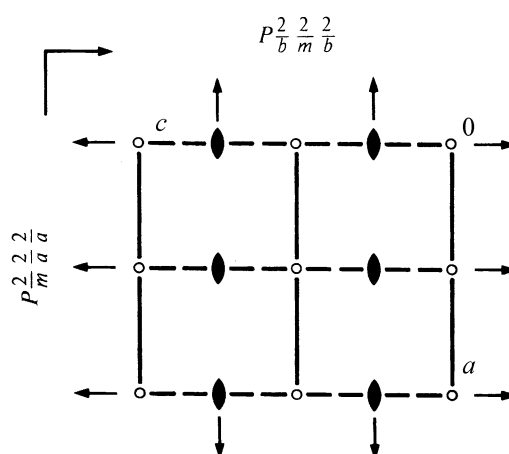
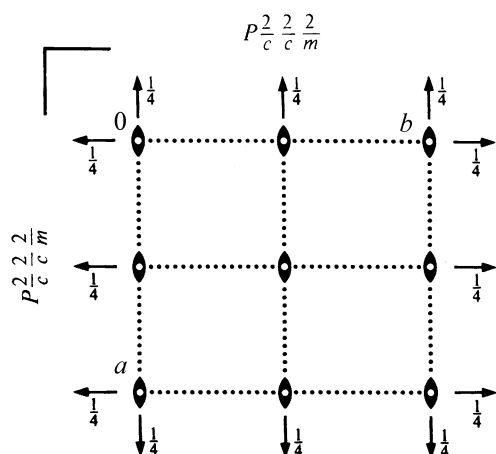
*mmm*

Orthorhombic

No. 49

*P 2/c 2/c 2/m*

Patterson symmetry *Pmmm*



**Origin** at centre ( $2/m$ ) at  $cc2/m$

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

**Symmetry operations**

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

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

**Positions**

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
8	<i>r</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) $\bar{x}, y, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y}, z + \frac{1}{2}$	(4) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y, z + \frac{1}{2}$	General: $0kl: l = 2n$ $h0l: l = 2n$ $00l: l = 2n$  Special: as above, plus no extra conditions
4	<i>q</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$	$hkl: l = 2n$
4	<i>p</i> .. 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl: l = 2n$
4	<i>o</i> .. 2	$0, \frac{1}{2}, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$0, \frac{1}{2}, z + \frac{1}{2}$	$hkl: l = 2n$
4	<i>n</i> .. 2	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: l = 2n$
4	<i>m</i> .. 2	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$	$hkl: l = 2n$
4	<i>l</i> .2.	$\frac{1}{2}, y, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{1}{4}$	$\frac{1}{2}, \bar{y}, \frac{3}{4}$	$\frac{1}{2}, y, \frac{3}{4}$	$hkl: l = 2n$
4	<i>k</i> .2.	$0, y, \frac{1}{4}$	$0, \bar{y}, \frac{1}{4}$	$0, \bar{y}, \frac{3}{4}$	$0, y, \frac{3}{4}$	$hkl: l = 2n$
4	<i>j</i> 2..	$x, \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \frac{1}{2}, \frac{1}{4}$	$\bar{x}, \frac{1}{2}, \frac{3}{4}$	$x, \frac{1}{2}, \frac{3}{4}$	$hkl: l = 2n$
4	<i>i</i> 2..	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$hkl: l = 2n$
2	<i>h</i> 222	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl: l = 2n$
2	<i>g</i> 222	$0, \frac{1}{2}, \frac{1}{4}$	$0, \frac{1}{2}, \frac{3}{4}$			$hkl: l = 2n$
2	<i>f</i> 222	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{3}{4}$			$hkl: l = 2n$
2	<i>e</i> 222	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl: l = 2n$
2	<i>d</i> .. 2/ <i>m</i>	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: l = 2n$
2	<i>c</i> .. 2/ <i>m</i>	$0, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl: l = 2n$
2	<i>b</i> .. 2/ <i>m</i>	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: l = 2n$
2	<i>a</i> .. 2/ <i>m</i>	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl: l = 2n$

**Symmetry of special projections**

Along [001]  $p2mm$

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

Origin at  $0, 0, z$

Along [100]  $p2mm$

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

Origin at  $x, 0, 0$

Along [010]  $p2mm$

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

Origin at  $0, y, 0$