

$Pn\bar{1}m$

$D_{2h}^{12}$

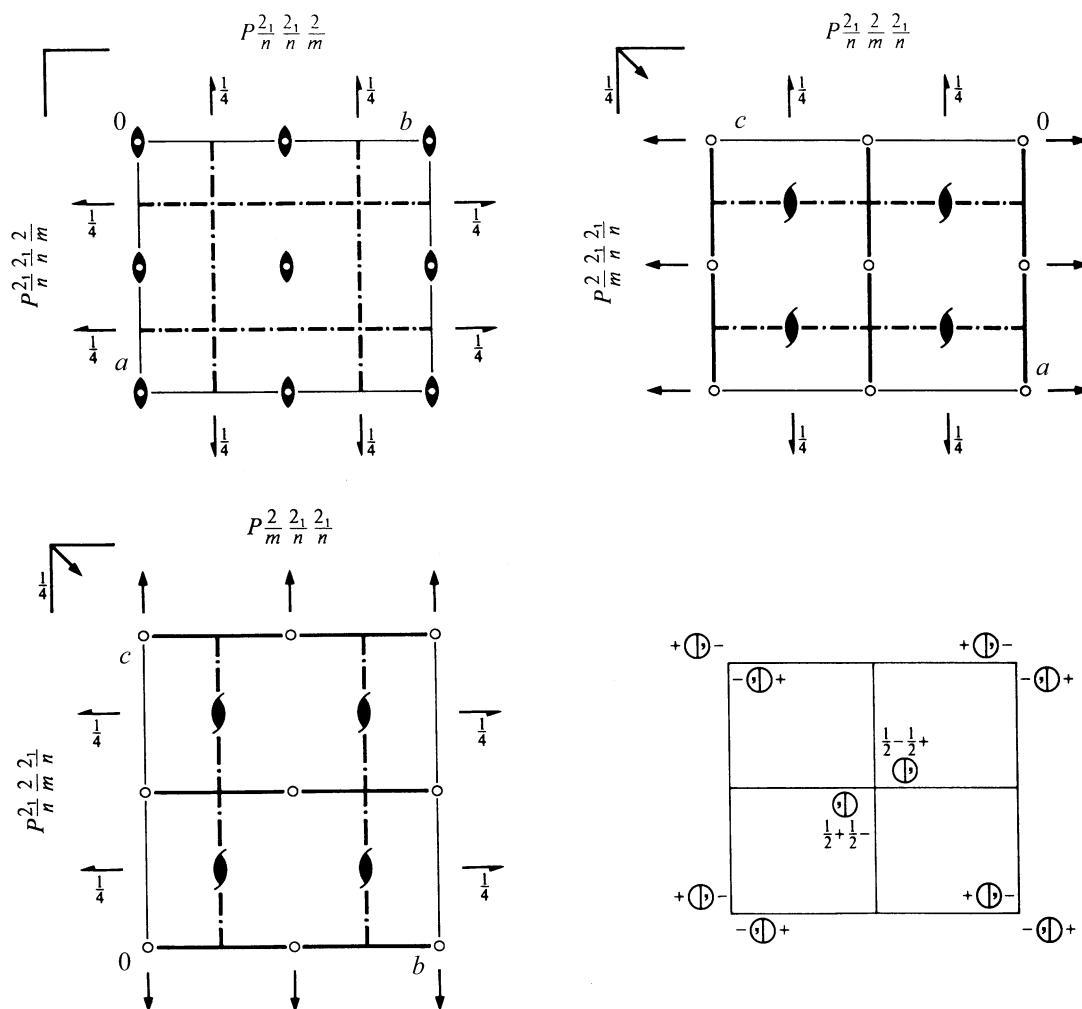
$mmm$

Orthorhombic

No. 58

$P 2_1/n 2_1/n 2/m$

Patterson symmetry  $Pmmm$



Origin at centre ( $2/m$ )

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

**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
					General:
8 <i>h</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) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$	$Ok\bar{l}: k + l = 2n$ $h0l: h + l = 2n$ $h00: h = 2n$ $0k0: k = 2n$ $00l: l = 2n$
4 <i>g</i> .. <i>m</i>	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$	Special: as above, plus no extra conditions
4 <i>f</i> .. 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
4 <i>e</i> .. 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$hkl: h + k + l = 2n$
2 <i>d</i> .. $2/m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl: h + k + l = 2n$
2 <i>c</i> .. $2/m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + k + l = 2n$
2 <i>b</i> .. $2/m$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$			$hkl: h + k + l = 2n$
2 <i>a</i> .. $2/m$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h + k + l = 2n$

**Symmetry of special projections**

Along [001]  $p2gg$

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

Origin at  $0, 0, z$

Along [100]  $c2mm$

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

Origin at  $x, 0, 0$

Along [010]  $c2mm$

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

Origin at  $0, y, 0$