

$Pmna$

D_{2h}^7

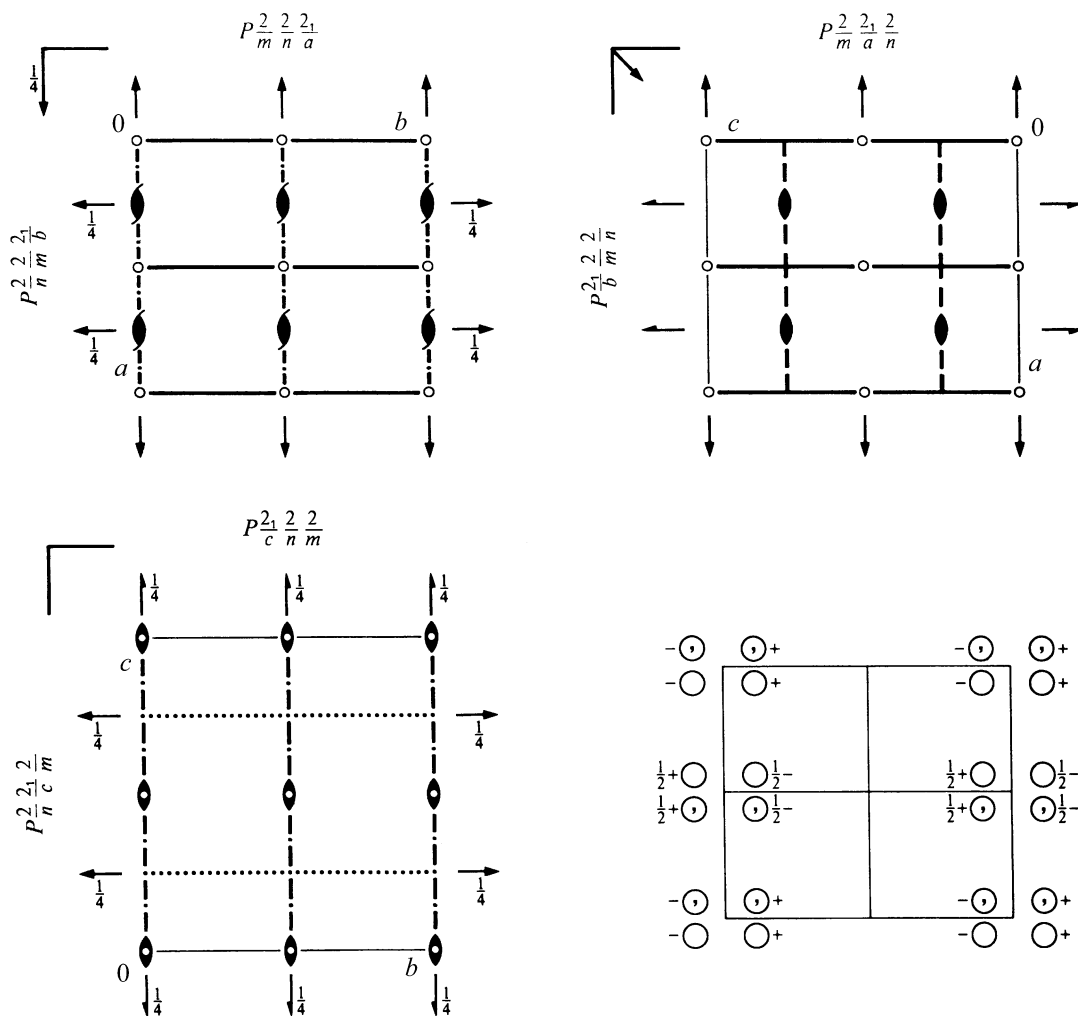
mmm

Orthorhombic

No. 53

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

Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $2/mn1$

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

Symmetry operations

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

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>i</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(4) x, \bar{y}, \bar{z} (8) \bar{x}, y, z	General: $h0l: h + l = 2n$ $hk0: h = 2n$ $h00: h = 2n$ $00l: l = 2n$ Special: as above, plus no extra conditions
4	<i>h</i> $m..$	$0, y, z$	$\frac{1}{2}, \bar{y}, z + \frac{1}{2}$	$\frac{1}{2}, y, \bar{z} + \frac{1}{2}$	$0, \bar{y}, \bar{z}$	no extra conditions
4	<i>g</i> $.2.$	$\frac{1}{4}, y, \frac{1}{4}$	$\frac{1}{4}, \bar{y}, \frac{3}{4}$	$\frac{3}{4}, \bar{y}, \frac{3}{4}$	$\frac{3}{4}, y, \frac{1}{4}$	$hkl: h = 2n$
4	<i>f</i> $2..$	$x, \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, 0$	$x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl: h + l = 2n$
4	<i>e</i> $2..$	$x, 0, 0$	$\bar{x} + \frac{1}{2}, 0, \frac{1}{2}$	$\bar{x}, 0, 0$	$x + \frac{1}{2}, 0, \frac{1}{2}$	$hkl: h + l = 2n$
2	<i>d</i> $2/m..$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl: h + l = 2n$
2	<i>c</i> $2/m..$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, \frac{1}{2}$			$hkl: h + l = 2n$
2	<i>b</i> $2/m..$	$\frac{1}{2}, 0, 0$	$0, 0, \frac{1}{2}$			$hkl: h + l = 2n$
2	<i>a</i> $2/m..$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + l = 2n$

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, 0, z$

Along [100] $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
 Origin at $0, y, 0$