

$Pmmn$

D_{2h}^{13}

mmm

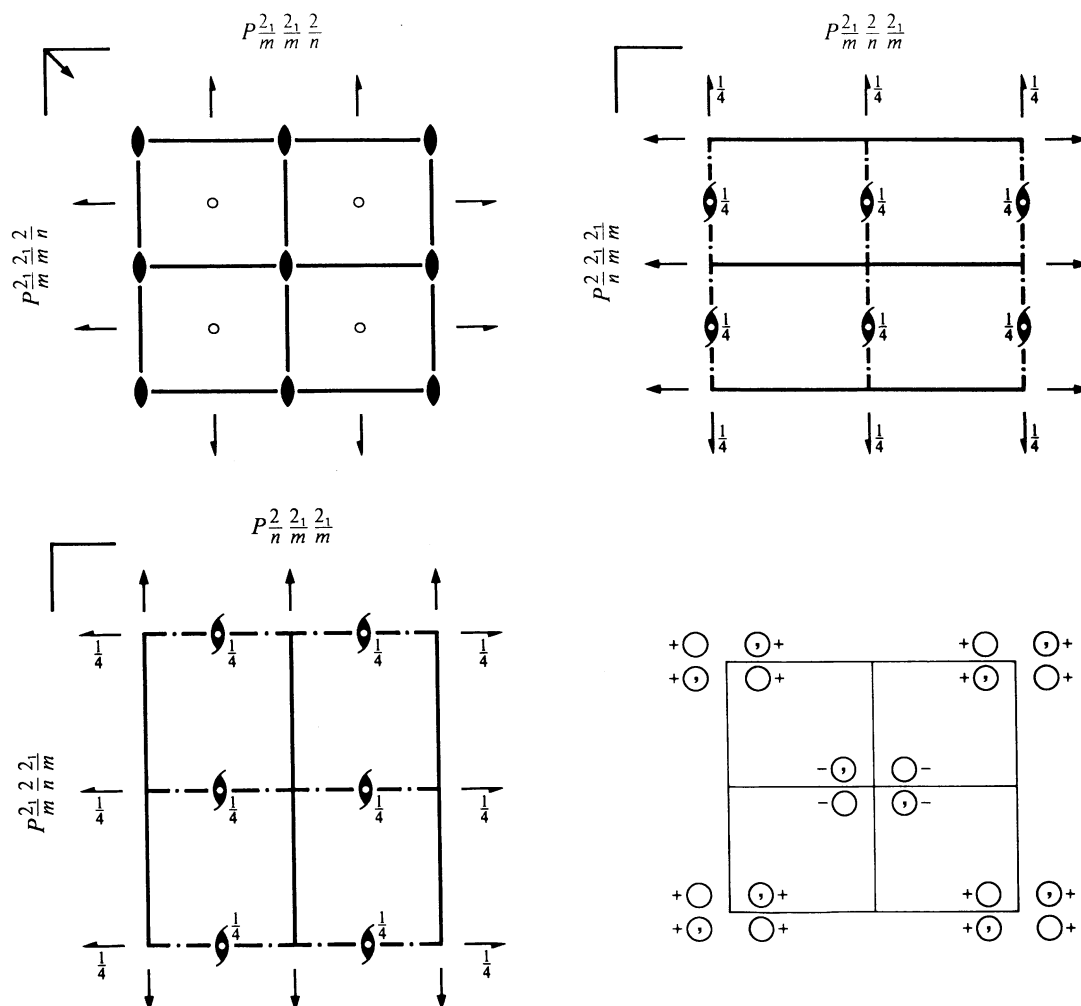
Orthorhombic

No. 59

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

Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $mm2/n$, at $\frac{1}{4}, \frac{1}{4}, 0$ from $\bar{1}$

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) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (4) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$ |
| (5) $\bar{1} \ \frac{1}{4}, \frac{1}{4}, 0$ | (6) $n(\frac{1}{2}, \frac{1}{2}, 0) \ x, y, 0$ | (7) $m \ x, 0, z$ | (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
					General:
8 <i>g</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (7) x, \bar{y}, z	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) \bar{x}, y, z	$hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
					Special: as above, plus
4 <i>f</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x} + \frac{1}{2}, \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \frac{1}{2}, \bar{z}$	no extra conditions
4 <i>e</i> <i>m</i> . .	$0, y, z$	$0, \bar{y}, z$	$\frac{1}{2}, y + \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$	no extra conditions
4 <i>d</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$hkl : h, k = 2n$
4 <i>c</i> $\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h, k = 2n$
2 <i>b</i> <i>m m</i> 2	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, \bar{z}$			no extra conditions
2 <i>a</i> <i>m m</i> 2	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$

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

Origin at 0, 0, z

Along [100] $p2mg$

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

Origin at $x, \frac{1}{4}, 0$

Along [010] $p2gm$

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

Origin at $\frac{1}{4}, y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pm2_1n$ ($Pmn2_1, 31$)	1; 3; 6; 8
	[2] $P2_1mn$ ($Pmn2_1, 31$)	1; 4; 6; 7
	[2] $Pmm2$ (25)	1; 2; 7; 8
	[2] $P2_12_12$ (18)	1; 2; 3; 4
	[2] $P112/n$ ($P2/c, 13$)	1; 2; 5; 6
	[2] $P12_1/m1$ ($P2_1/m, 11$)	1; 3; 5; 7
	[2] $P2_1/m11$ ($P2_1/m, 11$)	1; 4; 5; 8

IIa none

IIb [2] $Pcmn$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnma, 62$); [2] $Pm\bar{c}n$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pnma, 62$); [2] $Pccn$ ($\mathbf{c}' = 2\mathbf{c}$) (56)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pm\bar{m}n$ ($\mathbf{c}' = 2\mathbf{c}$) (59); [3] $Pm\bar{m}n$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

I [2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II [2] $Amma$ ($Cmcm, 63$); [2] $Bmmb$ ($Cmcm, 63$); [2] $Cmmm$ (65); [2] $Immm$ (71); [2] $Pmmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pmma, 51$); [2] $Pmma$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (51)