

$Pmmn$

D_{2h}^{13}

mmm

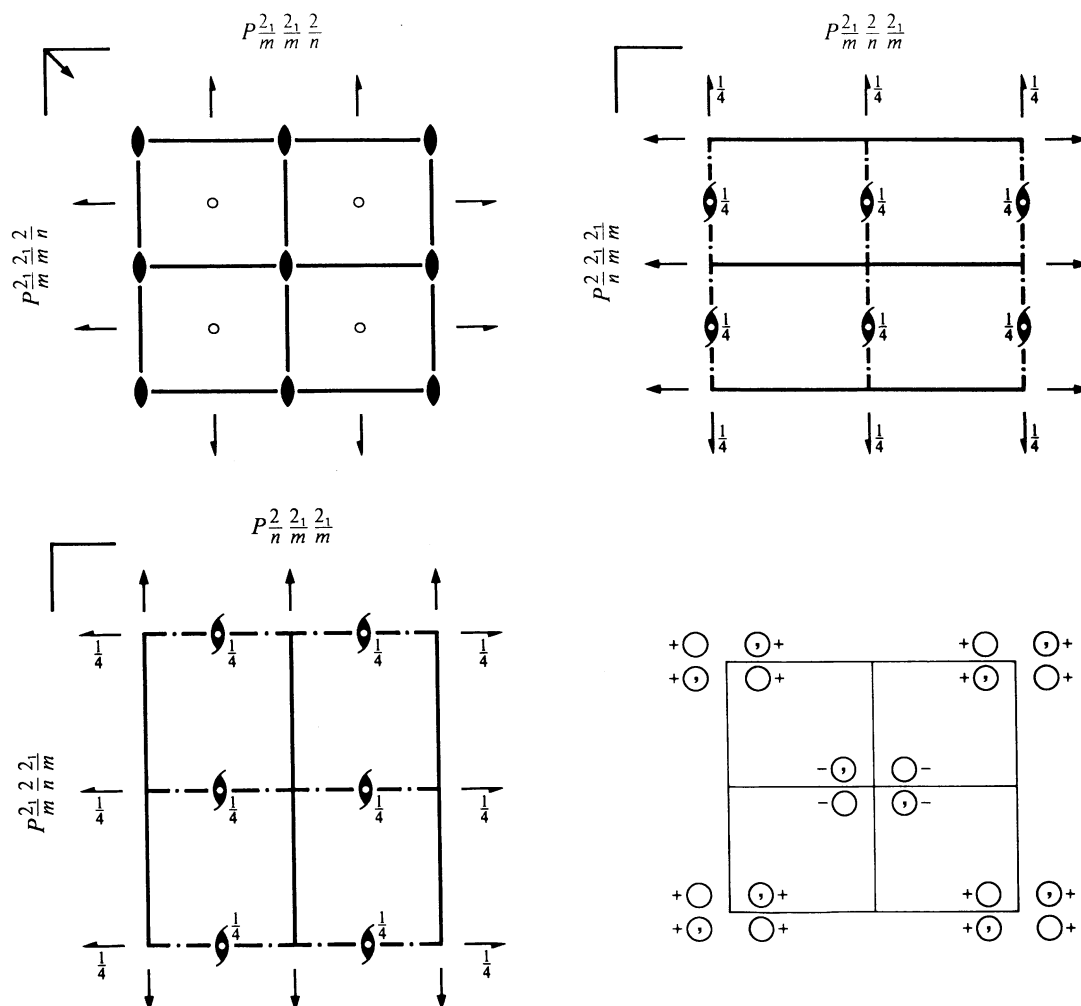
Orthorhombic

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
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	General: $hk0 : h + k = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ 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] *c*2*m m*

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

Origin at 0, 0, *z*

Along [100] *p*2*m g*

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

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

Along [010] *p*2*g m*

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

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

Maximal non-isomorphic subgroups

I	[2] <i>Pm</i> 2 ₁ <i>n</i> (<i>Pmn</i> 2 ₁ , 31)	1; 3; 6; 8
	[2] <i>P</i> 2 ₁ <i>mn</i> (<i>Pmn</i> 2 ₁ , 31)	1; 4; 6; 7
	[2] <i>Pmm</i> 2 (25)	1; 2; 7; 8
	[2] <i>P</i> 2 ₁ 2 ₁ 2 (18)	1; 2; 3; 4
	[2] <i>P</i> 112/ <i>n</i> (<i>P</i> 2/ <i>c</i> , 13)	1; 2; 5; 6
	[2] <i>P</i> 12 ₁ / <i>m</i> 1 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 3; 5; 7
	[2] <i>P</i> 2 ₁ / <i>m</i> 11 (<i>P</i> 2 ₁ / <i>m</i> , 11)	1; 4; 5; 8

IIa none

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

Maximal isomorphic subgroups of lowest index

IIc [2] *Pmmn* ($\mathbf{c}' = 2\mathbf{c}$) (59); [3] *Pmmn* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

I [2] *P*4/*nmm* (129); [2] *P*4₂/*nm**c* (137)

II [2] *A**mma* (*Cmcm*, 63); [2] *B**mmb* (*Cmcm*, 63); [2] *C**mmm* (65); [2] *I**mmm* (71); [2] *P**mmb* ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (*Pmma*, 51); [2] *P**mma* ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (51)

$Pmmn$

D_{2h}^{13}

mmm

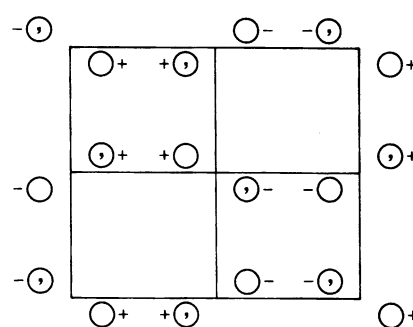
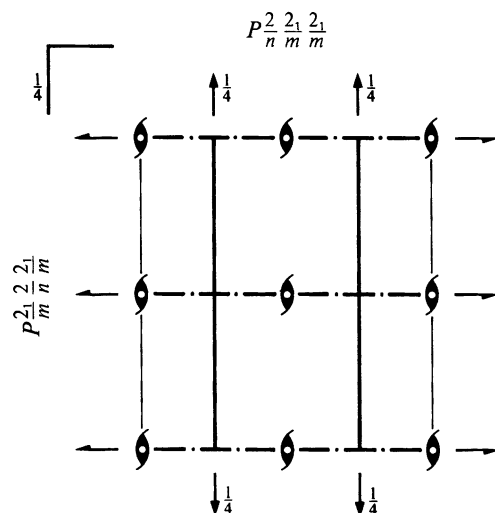
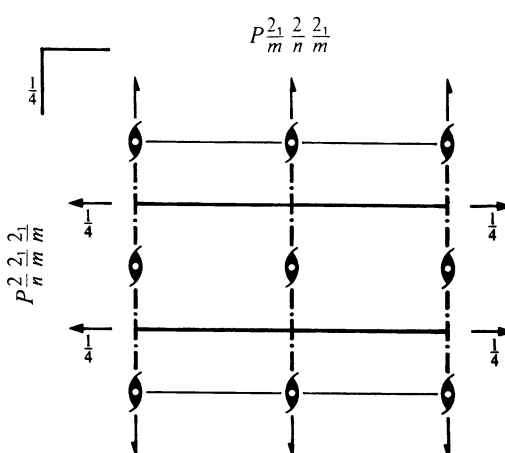
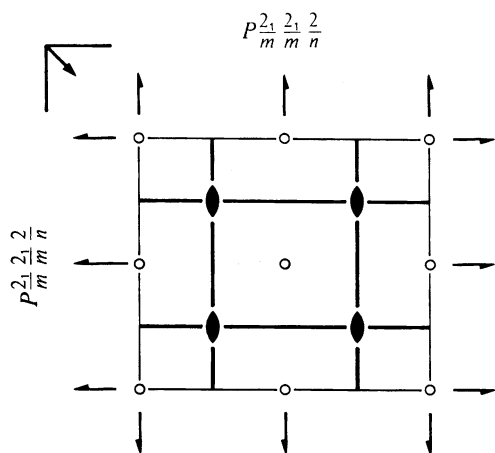
Orthorhombic

No. 59

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

Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $2_1 2_1 n$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from $mm2$

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

Symmetry operations

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

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

Symmetry of special projections

Along [001] *c2mm*

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

Origin at $\frac{1}{4}, \frac{1}{4}, z$

Along [100] *p2mg*

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

Origin at $x, 0, 0$

Along [010] *p2gm*

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

Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	[2] <i>Pm2₁n</i> (<i>Pmn2₁</i> , 31)	1; 3; 6; 8
	[2] <i>P2₁mn</i> (<i>Pmn2₁</i> , 31)	1; 4; 6; 7
	[2] <i>Pmm2</i> (25)	1; 2; 7; 8
	[2] <i>P2₁2₁2</i> (18)	1; 2; 3; 4
	[2] <i>P112/n</i> (<i>P2/c</i> , 13)	1; 2; 5; 6
	[2] <i>P12₁/m1</i> (<i>P2₁/m</i> , 11)	1; 3; 5; 7
	[2] <i>P2₁/m11</i> (<i>P2₁/m</i> , 11)	1; 4; 5; 8

IIa none

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

Maximal isomorphic subgroups of lowest index

IIc [2] *Pmmn* ($\mathbf{c}' = 2\mathbf{c}$) (59); [3] *Pmmn* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (59)

Minimal non-isomorphic supergroups

I [2] *P4/nmm* (129); [2] *P4₂/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)