

$Pmmn$

$D_{2h}^{13}$

$mmm$

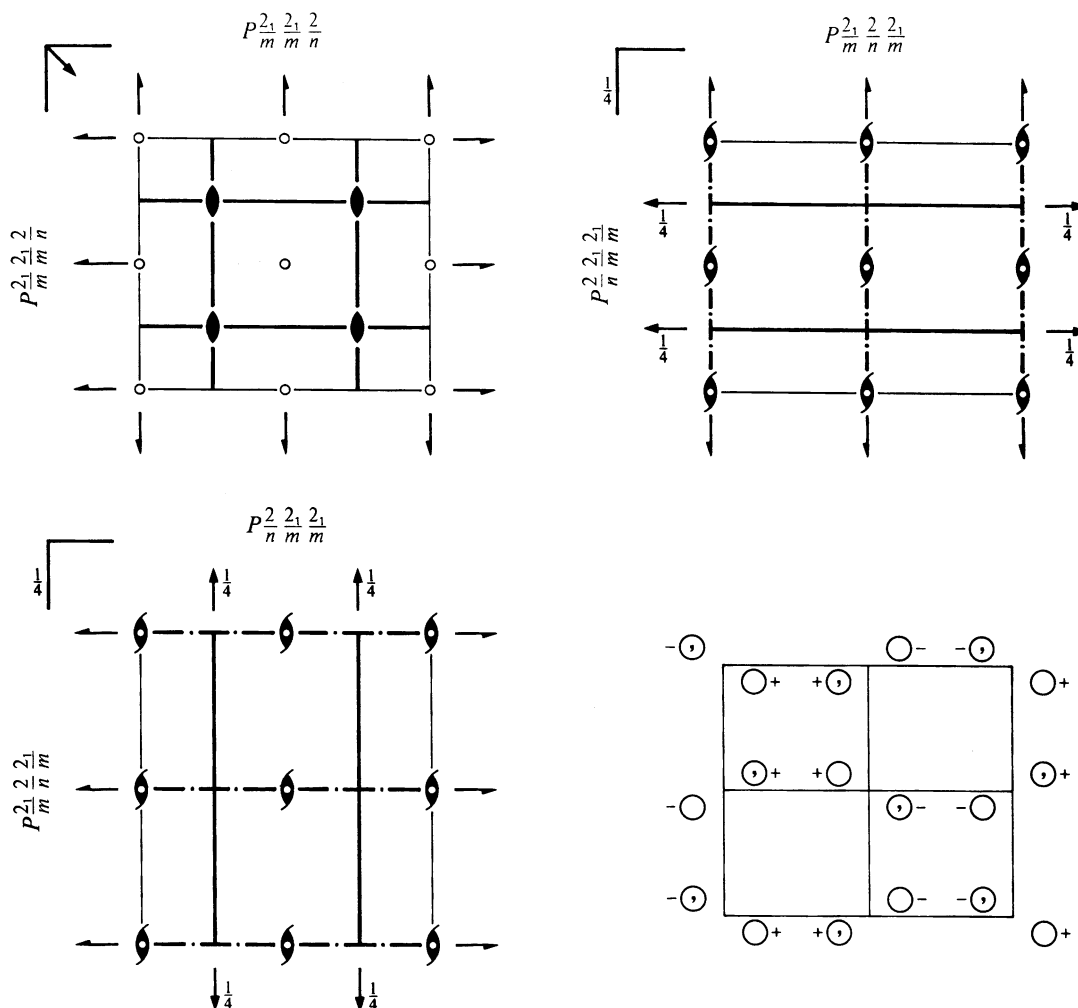
Orthorhombic

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**

<b>I</b>	[2] <i>Pm2<sub>1</sub>n</i> ( <i>Pmn2<sub>1</sub></i> , 31)	1; 3; 6; 8
	[2] <i>P2<sub>1</sub>mn</i> ( <i>Pmn2<sub>1</sub></i> , 31)	1; 4; 6; 7
	[2] <i>Pmm2</i> (25)	1; 2; 7; 8
	[2] <i>P2<sub>1</sub>2<sub>1</sub>2</i> (18)	1; 2; 3; 4
	[2] <i>P112/n</i> ( <i>P2/c</i> , 13)	1; 2; 5; 6
	[2] <i>P12<sub>1</sub>/m1</i> ( <i>P2<sub>1</sub>/m</i> , 11)	1; 3; 5; 7
	[2] <i>P2<sub>1</sub>/m11</i> ( <i>P2<sub>1</sub>/m</i> , 11)	1; 4; 5; 8

**IIa** none

**IIb** [2] *Pcmn* ( $\mathbf{c}' = 2\mathbf{c}$ ) (*Pnma*, 62); [2] *Pm<sub>2</sub>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] *P4/nmm* (129); [2] *P4<sub>2</sub>/nmc* (137)

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