

$Pnna$

$D_{2h}^6$

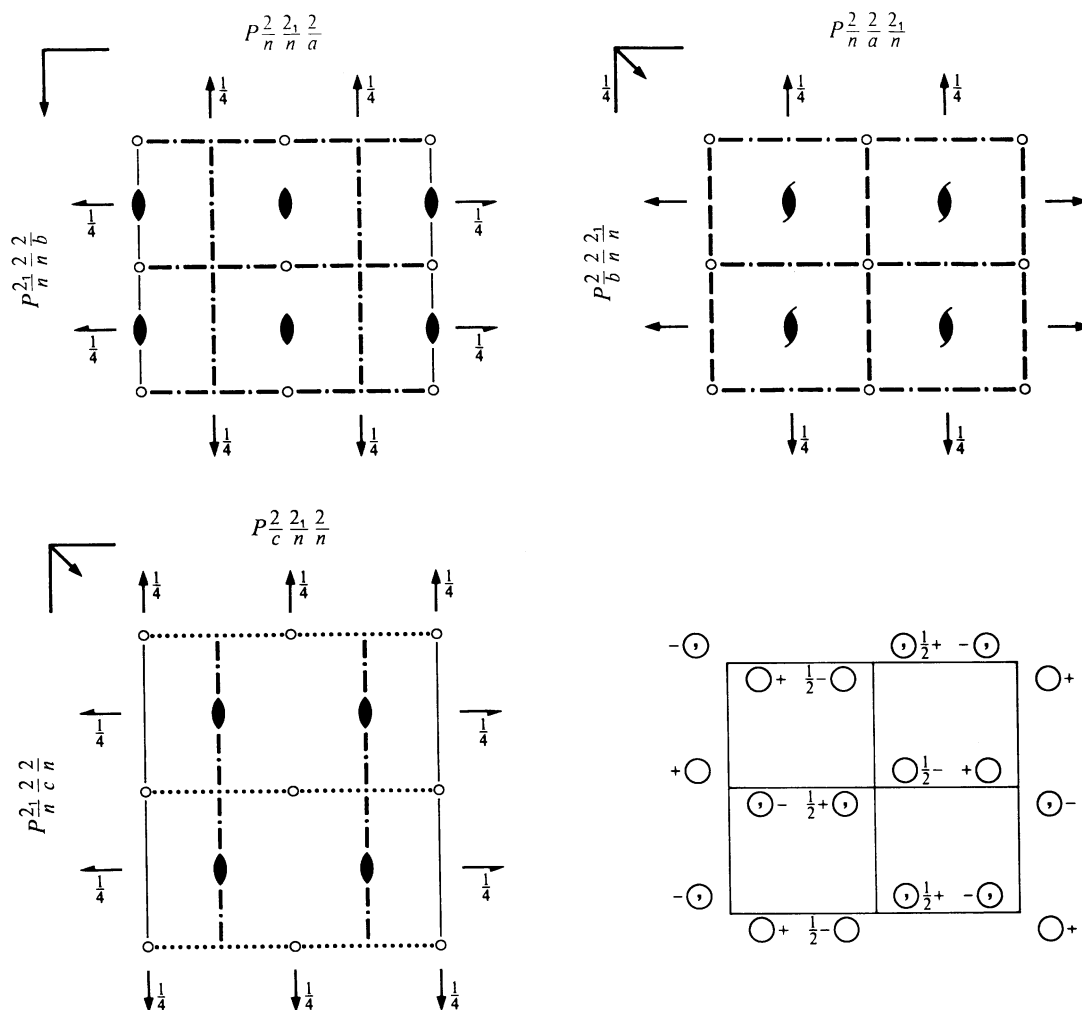
$mmm$

Orthorhombic

No. 52

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

Patterson symmetry  $Pmmm$



Origin at  $\bar{1}$  on  $n1a$

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

Symmetry operations

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

**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>e</i> 1	(1) $x, y, z$ (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ (6) $x + \frac{1}{2}, y, \bar{z}$	(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) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (8) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$	General: $Ok\bar{l} : k + l = 2n$ $h0l : h + l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$  Special: as above, plus $hkl : h + l = 2n$ $hkl : h + k + l = 2n$ $hkl : h, k + l = 2n$ $hkl : h, k + l = 2n$
4 <i>d</i> 2..	$x, \frac{1}{4}, \frac{1}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\bar{x}, \frac{3}{4}, \frac{3}{4}$	$x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$	$hkl : h + l = 2n$
4 <i>c</i> ..2	$\frac{1}{4}, 0, z$	$\frac{1}{4}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{3}{4}, 0, \bar{z}$	$\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}$	$hkl : h + k + l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$0, \frac{1}{2}, 0$	$hkl : h, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$hkl : h, k + l = 2n$

**Symmetry of special projections**

Along [001]  $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 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  $\frac{1}{4}, y, \frac{1}{4}$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $Pnn2$ (34)	1; 2; 7; 8
	[2] $Pn2_1a$ ( $Pna2_1$ , 33)	1; 3; 6; 8
	[2] $P2na$ ( $Pnc2$ , 30)	1; 4; 6; 7
	[2] $P22_12$ ( $P222_1$ , 17)	1; 2; 3; 4
	[2] $P12_1/n1$ ( $P2_1/c$ , 14)	1; 3; 5; 7
	[2] $P112/a$ ( $P2/c$ , 13)	1; 2; 5; 6
	[2] $P2/n11$ ( $P2/c$ , 13)	1; 4; 5; 8

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $Pnna$  ( $\mathbf{a}' = 3\mathbf{a}$ ) (52); [3]  $Pnna$  ( $\mathbf{b}' = 3\mathbf{b}$ ) (52); [3]  $Pnna$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (52)

**Minimal non-isomorphic supergroups**

**I** none

**II** [2]  $Bbmm$  ( $Cmcm$ , 63); [2]  $Amaa$  ( $Cccm$ , 66); [2]  $Ccce$  (68); [2]  $Imma$  (74); [2]  $Pncm$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pmna$ , 53); [2]  $Pcna$  ( $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ) ( $Pban$ , 50); [2]  $Pbaa$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $Pcca$ , 54)