

$Pnna$

$D_{2h}^6$

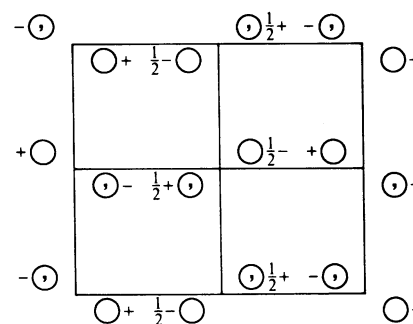
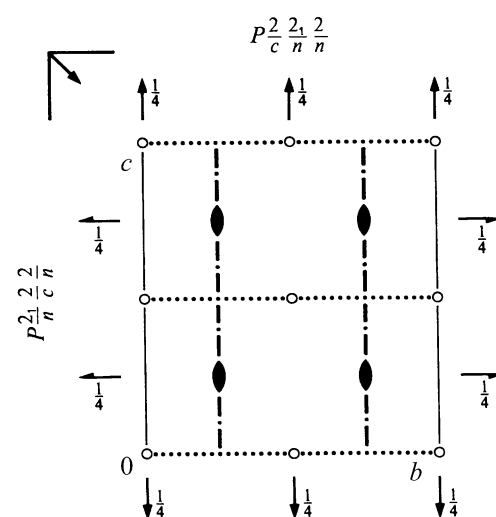
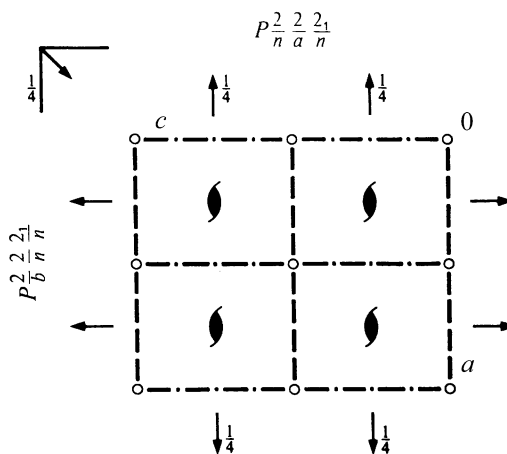
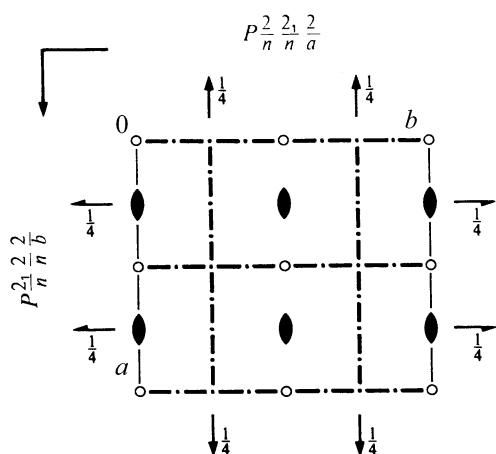
$mmm$

Orthorhombic

No. 52

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

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 $\frac{1}{4}, 0, z$ | (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

		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: $Ok\bar{l}: k + l = 2n$ $h0\bar{l}: h + l = 2n$ $hk0: h = 2n$ $h00: h = 2n$ $0k0: k = 2n$ $00\bar{l}: l = 2n$  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  $\frac{1}{4}, y, \frac{1}{4}$