

*Pbca*

$D_{2h}^{15}$

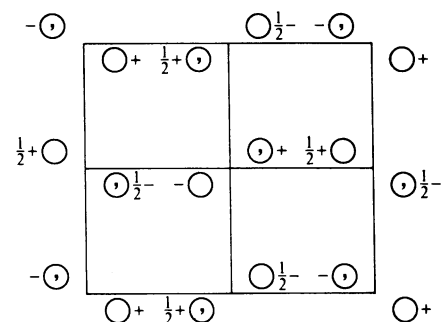
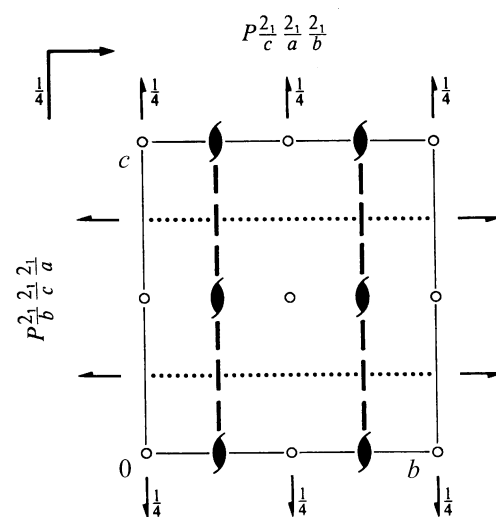
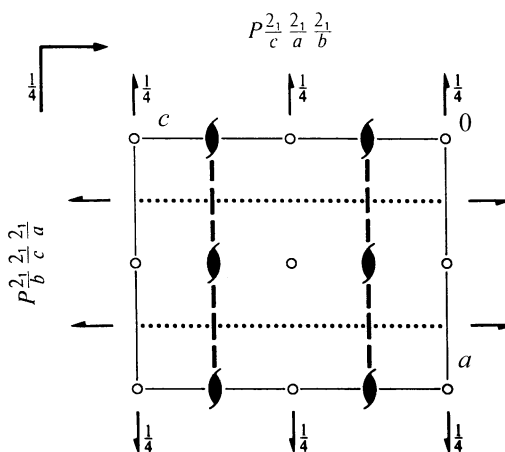
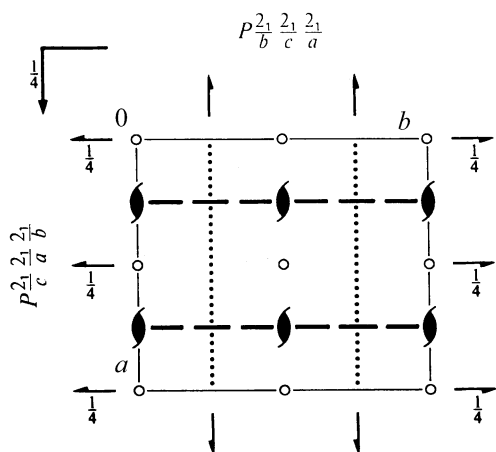
*mmm*

Orthorhombic

No. 61

$P 2_1/b 2_1/c 2_1/a$

Patterson symmetry *Pmmm*



Origin at  $\bar{1}$

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

**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>c</i>	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$

General:

$0kl$ :  $k = 2n$   
 $h0l$ :  $l = 2n$   
 $hk0$ :  $h = 2n$   
 $h00$ :  $h = 2n$   
 $0k0$ :  $k = 2n$   
 $00l$ :  $l = 2n$

Special: as above, plus

4	<i>b</i>	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
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 $hkl$ :  $h + k, h + l, k + l = 2n$ 

4	<i>a</i>	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
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 $hkl$ :  $h + k, h + l, k + l = 2n$ **Symmetry of special projections**

Along  $[001]$   $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$      $\mathbf{b}' = \mathbf{b}$   
 Origin at  $0, 0, z$

Along  $[100]$   $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$      $\mathbf{b}' = \mathbf{c}$   
 Origin at  $x, 0, 0$

Along  $[010]$   $p2gm$   
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$      $\mathbf{b}' = \mathbf{a}$   
 Origin at  $0, y, 0$