

Pbca

D_{2h}^{15}

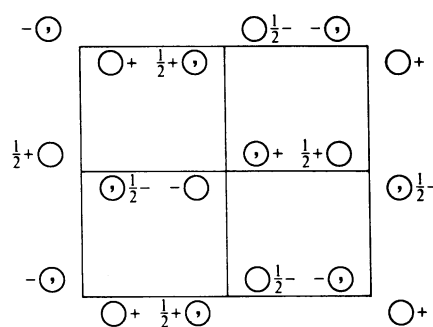
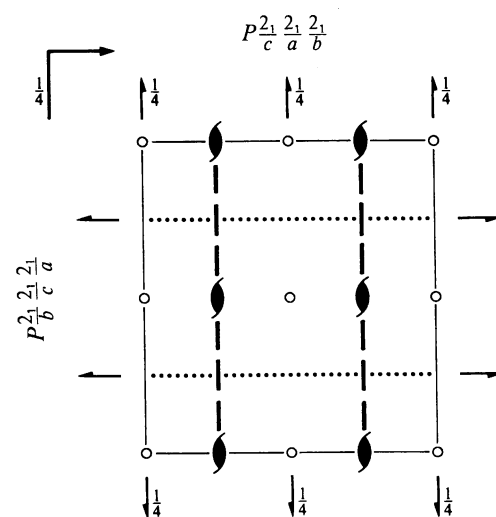
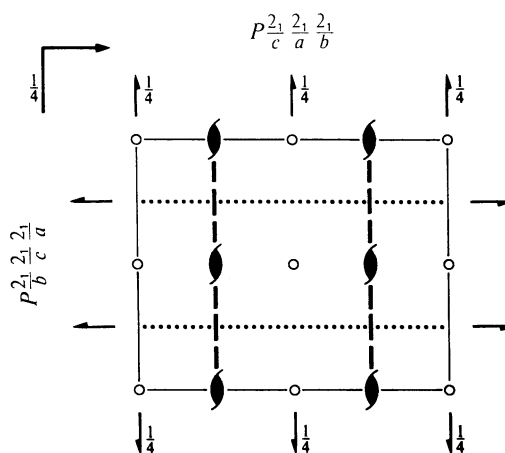
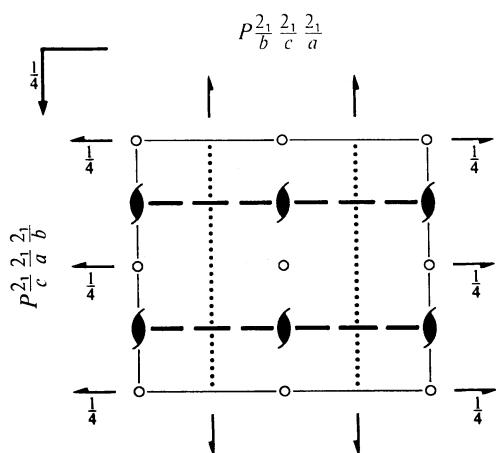
mmm

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 (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	General: $Ok\bar{l} : k = 2n$ $h0l : l = 2n$ $hk0 : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus $hkl : h + k, h + l, k + l = 2n$ $hkl : h + k, h + l, k + l = 2n$
4 <i>b</i> $\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k, h + l, k + l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k, h + l, k + l = 2n$

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, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $Pbc2_1 (Pca2_1, 29)$	1; 2; 7; 8
	[2] $Pb2_1a (Pca2_1, 29)$	1; 3; 6; 8
	[2] $P2_1ca (Pca2_1, 29)$	1; 4; 6; 7
	[2] $P2_12_12_1 (19)$	1; 2; 3; 4
	[2] $P112_1/a (P2_1/c, 14)$	1; 2; 5; 6
	[2] $P12_1/c1 (P2_1/c, 14)$	1; 3; 5; 7
	[2] $P2_1/b11 (P2_1/c, 14)$	1; 4; 5; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbca (\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}) (61)$

Minimal non-isomorphic supergroups

I [3] $Pa\bar{3} (205)$

II [2] $Aema (Cmce, 64)$; [2] $Bbem (Cmce, 64)$; [2] $Cmce (64)$; [2] $Ibca (73)$; [2] $Pbcm (\mathbf{a}' = \frac{1}{2}\mathbf{a}) (57)$;
 [2] $Pmca (\mathbf{b}' = \frac{1}{2}\mathbf{b}) (Pbcm, 57)$; [2] $Pbma (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (Pbcm, 57)$