

$Pbcm$

D_{2h}^{11}

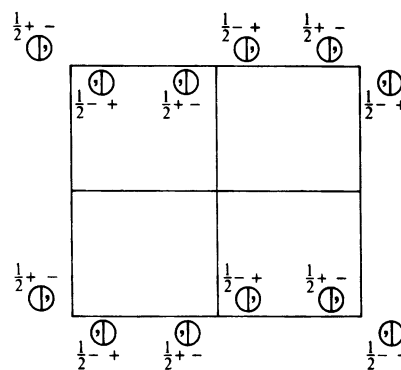
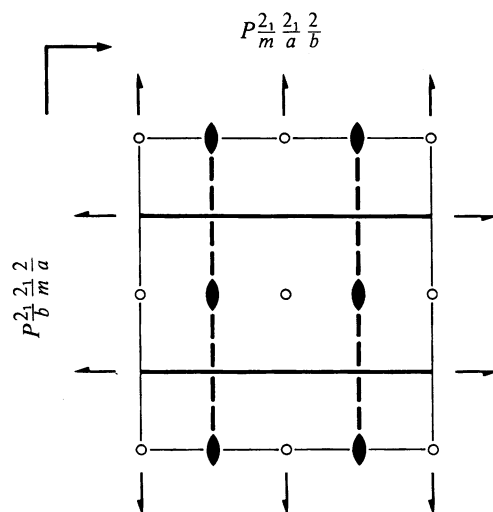
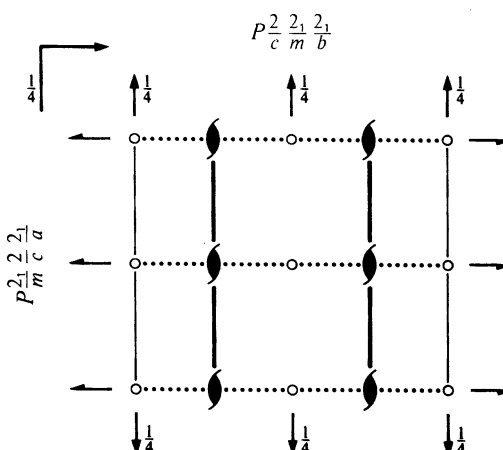
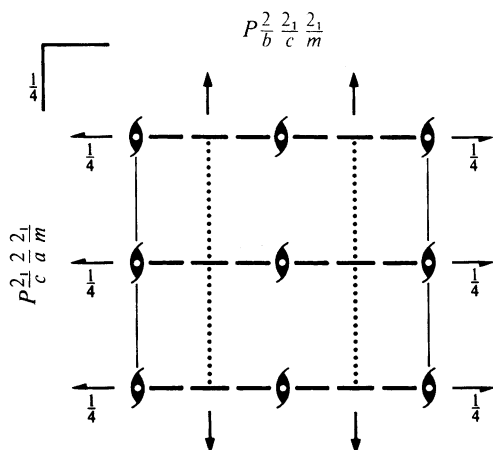
mmm

Orthorhombic

No. 57

$P 2/b 2_1/c 2_1/m$

Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $b12_1$

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

Symmetry operations

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

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) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x, y, \bar{z} + \frac{1}{2}$	(3) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (8) $\bar{x}, y + \frac{1}{2}, z$	General: $0kl : k = 2n$ $h0l : l = 2n$ $0k0 : k = 2n$ $00l : l = 2n$ Special: as above, plus
4 <i>d</i> $\dots m$	$x, y, \frac{1}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$	$\bar{x}, y + \frac{1}{2}, \frac{1}{4}$	$x, \bar{y} + \frac{1}{2}, \frac{3}{4}$	no extra conditions
4 <i>c</i> $2 \dots$	$x, \frac{1}{4}, 0$	$\bar{x}, \frac{3}{4}, \frac{1}{2}$	$\bar{x}, \frac{1}{4}, 0$	$x, \frac{1}{4}, \frac{1}{2}$	$hkl : l = 2n$
4 <i>b</i> $\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : k, l = 2n$
4 <i>a</i> $\bar{1}$	$0, 0, 0$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$hkl : k, l = 2n$

Symmetry of special projections

Along [001] $p2gm$

$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

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] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$

Origin at 0, y, 0

Maximal non-isomorphic subgroups

I	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2cm$ ($Pma2$, 28)	1; 4; 6; 7
	[2] $Pb2_1m$ ($Pmc2_1$, 26)	1; 3; 6; 8
	[2] $P22_12_1$ ($P2_12_12_1$, 18)	1; 2; 3; 4
	[2] $P12_1/c1$ ($P2_1/c$, 14)	1; 3; 5; 7
	[2] $P2/b11$ ($P2/c$, 13)	1; 4; 5; 8
	[2] $P112_1/m$ ($P2_1/m$, 11)	1; 2; 5; 6

IIa none

IIb [2] $Pbnm$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pnma$, 62); [2] $Pbca$ ($\mathbf{a}' = 2\mathbf{a}$) (61); [2] $Pbna$ ($\mathbf{a}' = 2\mathbf{a}$) ($Pbcn$, 60)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pbcm$ ($\mathbf{a}' = 2\mathbf{a}$) (57); [3] $Pbcm$ ($\mathbf{b}' = 3\mathbf{b}$) (57); [3] $Pbcm$ ($\mathbf{c}' = 3\mathbf{c}$) (57)

Minimal non-isomorphic supergroups

I none

II [2] $Cmcm$ (63); [2] $Bbem$ ($Cmce$, 64); [2] $Aemm$ ($Cmme$, 67); [2] $Ibam$ (72); [2] $Pmcm$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Pbmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pmma$, 51)