

*Pba*2

C_{2v}^8

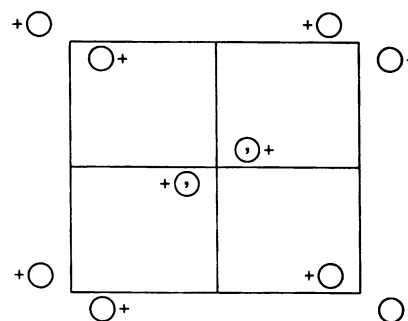
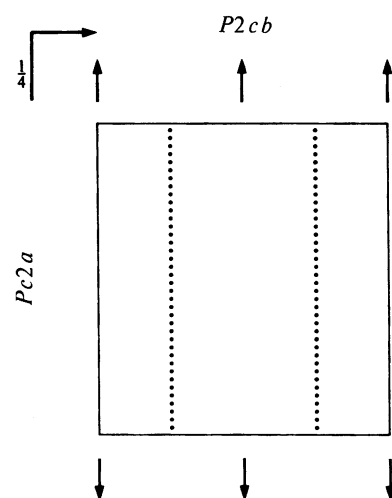
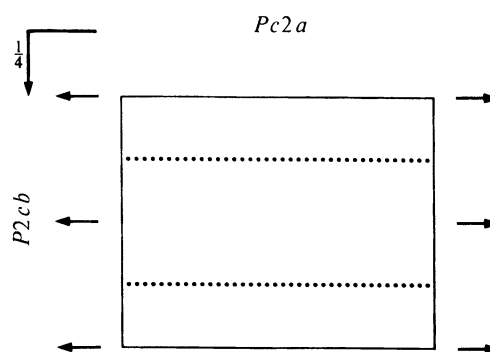
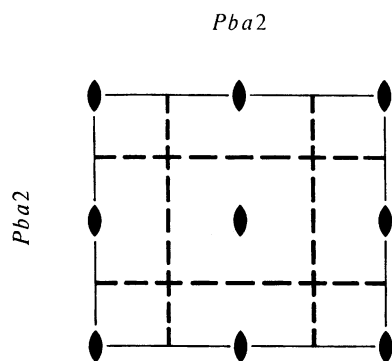
*mm*2

Orthorhombic

No. 32

*Pba*2

Patterson symmetry *Pmmm*



Origin on 112

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

Symmetry operations

- (1) 1 (2) 2 $0, 0, z$ (3) *a* $x, \frac{1}{4}, z$ (4) *b* $\frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 <i>c</i> 1	(1) x,y,z	(2) \bar{x},\bar{y},z	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl : k = 2n$ $h0l : h = 2n$ $h00 : h = 2n$ $0k0 : k = 2n$
2 <i>b</i> .. 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			Special: as above, plus $hkl : h+k = 2n$
2 <i>a</i> .. 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			$hkl : h+k = 2n$

Symmetry of special projections

Along [001] $p2gg$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at 0, 0, z

Along [100] $p1m1$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $p11m$
 $\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0, y, 0

Maximal non-isomorphic subgroups

I [2] $P1a1$ (Pc , 7) 1; 3
 [2] $Pb11$ (Pc , 7) 1; 4
 [2] $P112$ ($P2$, 3) 1; 2

IIa none

IIb [2] $Pnn2$ ($\mathbf{c}' = 2\mathbf{c}$) (34); [2] $Pna2_1$ ($\mathbf{c}' = 2\mathbf{c}$) (33); [2] $Pbn2_1$ ($\mathbf{c}' = 2\mathbf{c}$) ($Pna2_1$, 33)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pba2$ ($\mathbf{c}' = 2\mathbf{c}$) (32); [3] $Pba2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (32)

Minimal non-isomorphic supergroups

I [2] $Pban$ (50); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $P4bm$ (100); [2] $P4_2bc$ (106); [2] $P\bar{4}b2$ (117)

II [2] $Cmm2$ (35); [2] $Aea2$ (41); [2] $Bbe2$ ($Aea2$, 41); [2] $Iba2$ (45); [2] $Pbm2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pma2$, 28); [2] $Pma2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (28)