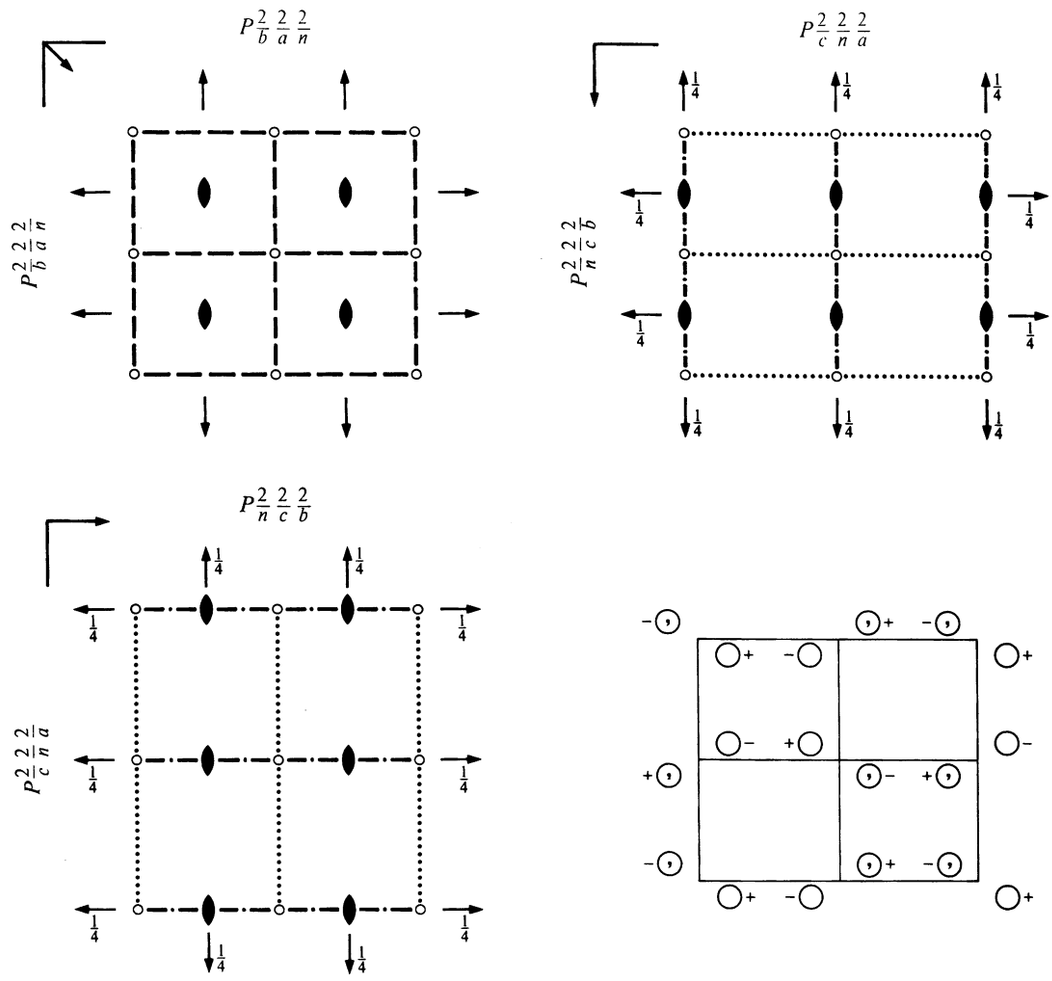
International Tables for Crystallography (2006). Vol. A, Space group 50, pp. 272–273.

$Pban$ D_{2h}^{4} mmm Orthorhombic

No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at ban, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from 222

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

Symmetry operations

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

Minimal non-isomorphic supergroups

I [2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II [2] $Cmmm$ (65); [2] $Aeaa$ ($Ccce$, 68); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pccm$, 49); [2] $Pmaa$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pccm$, 49)

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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
							General:
8	m	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x+\frac{1}{2},\bar{y},z$	(8) $\bar{x},y+\frac{1}{2},z$	$h0l$: $h=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							Special: as above, plus
4	l	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z$	hkl : $h+k=2n$
4	k	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	hkl : $h+k=2n$
4	j	. 2 .	$\frac{1}{4},y,\frac{1}{2}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},y+\frac{1}{2},\frac{1}{2}$	hkl : $h+k=2n$
4	i	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y+\frac{1}{2},0$	hkl : $h+k=2n$
4	h	2 . .	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	hkl : $h+k=2n$
4	g	2 . .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	hkl : $h+k=2n$
4	f	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h,k=2n$
4	e	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl : $h,k=2n$
2	d	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	c	2 2 2	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl : $h+k=2n$
2	b	2 2 2	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl : $h+k=2n$
2	a	2 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $Pba2$ (32) 1; 2; 7; 8
[2] $Pb2n$ ($Pnc2$, 30) 1; 3; 6; 8
[2] $P2an$ ($Pnc2$, 30) 1; 4; 6; 7
[2] $P222$ (16) 1; 2; 3; 4
[2] $P112/n$ ($P2/c$, 13) 1; 2; 5; 6
[2] $P12/a1$ ($P2/c$, 13) 1; 3; 5; 7
[2] $P2/b11$ ($P2/c$, 13) 1; 4; 5; 8

IIa none

IIb [2] $Pnan$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pbnn$ ($\mathbf{c}'=2\mathbf{c}$) ($Pnna$, 52); [2] $Pnnn$ ($\mathbf{c}'=2\mathbf{c}$) (48)

Maximal isomorphic subgroups of lowest index

IIc [2] $Pban$ ($\mathbf{c}'=2\mathbf{c}$) (50); [3] $Pban$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$) (50)

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