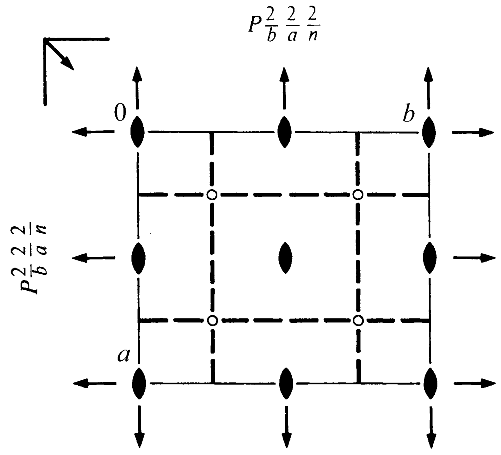
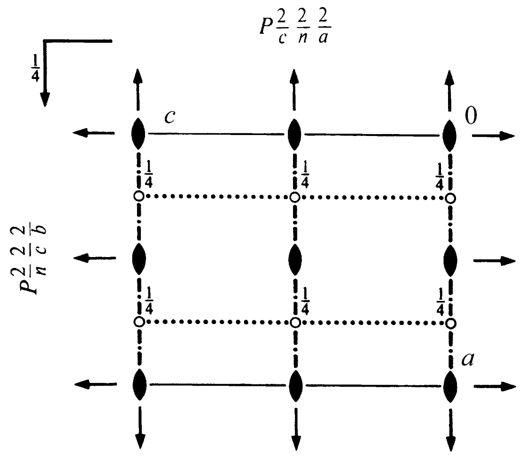
International Tables for Crystallography (2016). Vol. A, Space group 50, pp. 326–329.

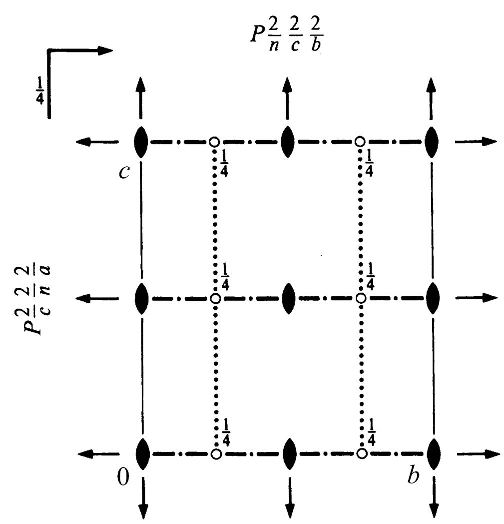
Pban D_{2h}^4 *mmm* Orthorhombic

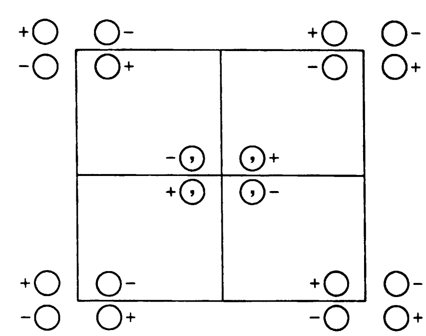
No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1









Origin at $222/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

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

Symmetry operations

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

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

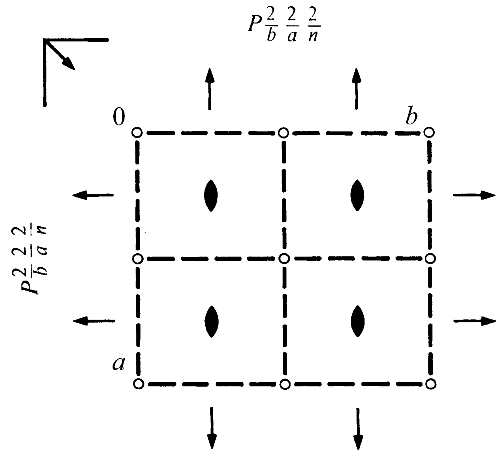
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

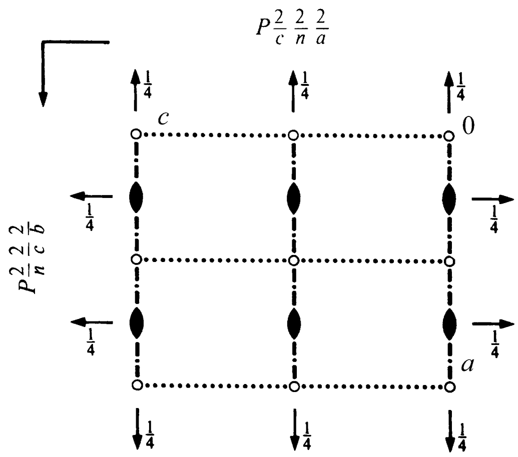
Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

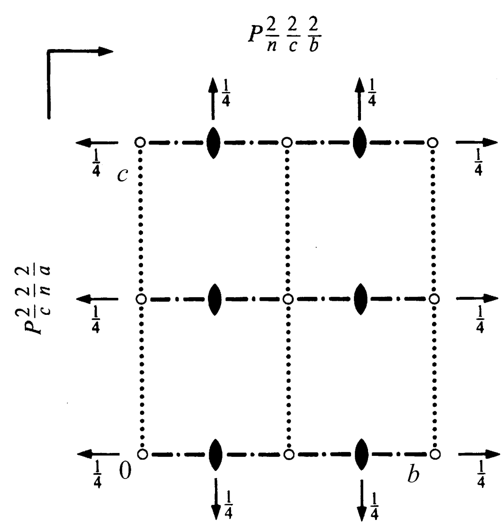
Pban D_{2h}^4 *mmm* Orthorhombic

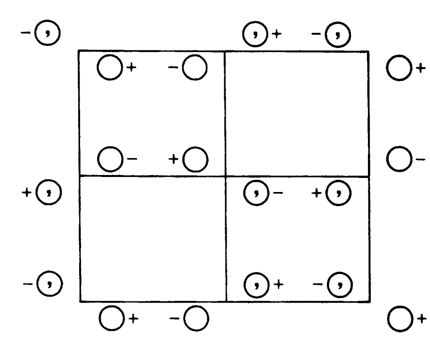
No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 2









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

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

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 $0,y,z$

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 (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y},z$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							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 $0,y,0$