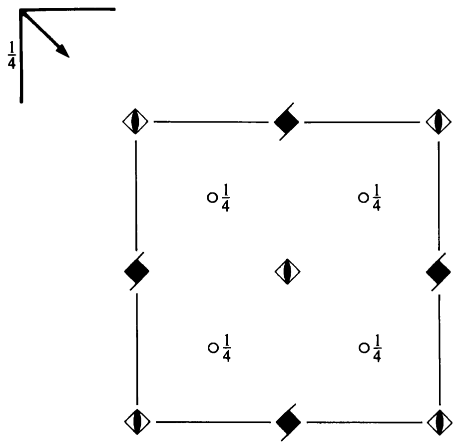
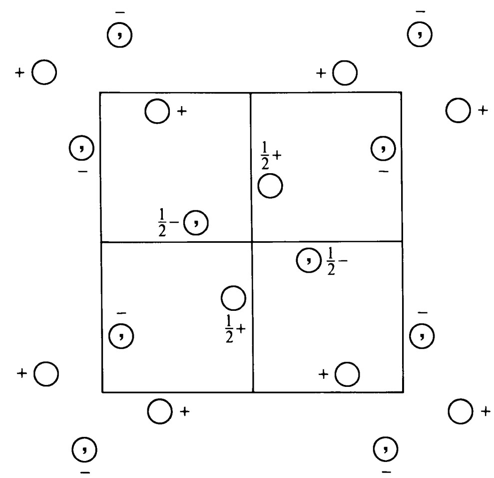
International Tables for Crystallography (2016). Vol. A, Space group 86, pp. 396–397.

$P4_2/n$ $\quad C_{4h}^4$ $\quad 4/m$ $\quad$ Tetragonal

No. 86 $\quad P4_2/n$ $\quad$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1





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

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

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $\bar{1}\quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)\quad x,y,\frac{1}{4}$	(7) $\bar{4}^+\ 0,0,z;\ 0,0,0$	(8) $\bar{4}^-\ 0,0,z;\ 0,0,0$

Generators selected $\quad (1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ (2);\ (3);\ (5)$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
4	e	$2\,.\,.$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
2	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

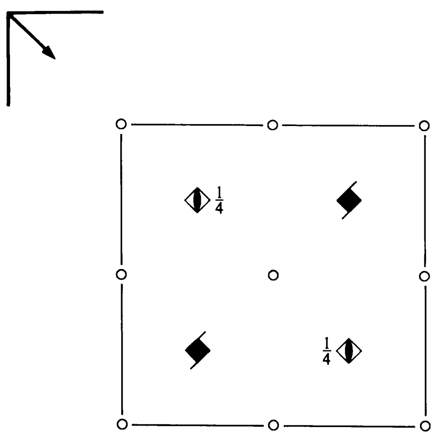
Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

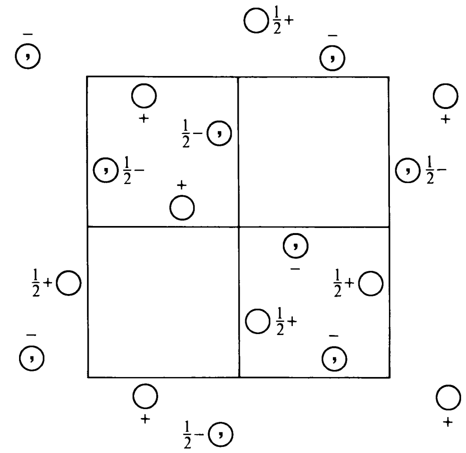
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

Copyright © 2016 International Union of Crystallography

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

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

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(8) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

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	g	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) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	f	$2\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	e	$2\,.\,.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
2	b	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h+k+l=2n$
2	a	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$