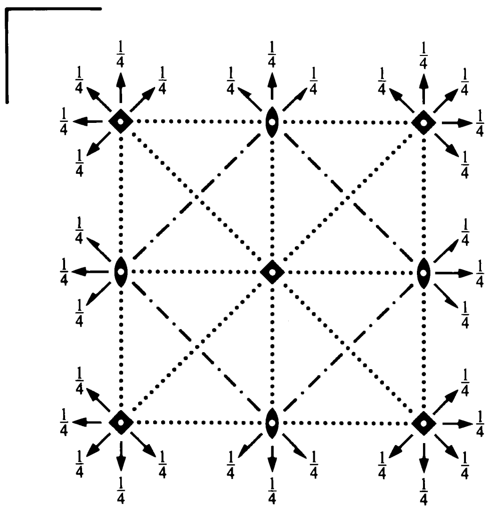
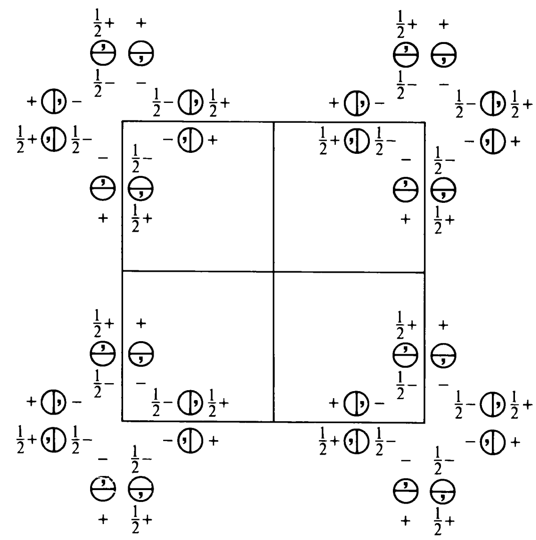
International Tables for Crystallography (2016). Vol. A, Space group 124, pp. 444–445.

$P4/mcc$ $\quad D_{4h}^{2}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 124 $\quad P\ 4/m\ 2/c\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/mcc$

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

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,0,z$	(4) $4^{-}\quad 0,0,z$
(5) $2\quad 0,y,\frac{1}{4}$	(6) $2\quad x,0,\frac{1}{4}$	(7) $2\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^{+}\quad 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^{-}\quad 0,0,z;\ \ 0,0,0$
(13) $c\quad x,0,z$	(14) $c\quad 0,y,z$	(15) $c\quad x,\bar{x},z$	(16) $c\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	*n*	1	(1) x,y,z (5) $\bar{x},y,\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}$ (16) $y,x,z+\frac{1}{2}$	$0kl$: $l=2n$ hhl: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*m*	$m\,.\,.$	$x,y,0$ $\bar{x},y,\frac{1}{2}$	$\bar{x},\bar{y},0$ $x,\bar{y},\frac{1}{2}$	$\bar{y},x,0$ $y,x,\frac{1}{2}$	$y,\bar{x},0$ $\bar{y},\bar{x},\frac{1}{2}$	no extra conditions
8	*l*	$.\,2\,.$	$x,\frac{1}{2},\frac{1}{4}$ $\bar{x},\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$ $x,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},x,\frac{1}{4}$ $\frac{1}{2},\bar{x},\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{1}{4}$ $\frac{1}{2},x,\frac{3}{4}$	hkl: $l=2n$
8	*k*	$.\,2\,.$	$x,0,\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$	$\bar{x},0,\frac{1}{4}$ $x,0,\frac{3}{4}$	$0,x,\frac{1}{4}$ $0,\bar{x},\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$ $0,x,\frac{3}{4}$	hkl: $l=2n$
8	*j*	$.\,.\,2$	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},\bar{x},\frac{1}{4}$ $x,x,\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$	hkl: $l=2n$
8	*i*	$2\,.\,.$	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$ $\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$	hkl: $h+k,l=2n$
4	*h*	$4\,.\,.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	*g*	$4\,.\,.$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
4	*f*	$2\,2\,2\,.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	*e*	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,l=2n$
2	*d*	$4/m\,.\,.$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	*c*	$4\,2\,2$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	*b*	$4/m\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
2	*a*	$4\,2\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

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

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