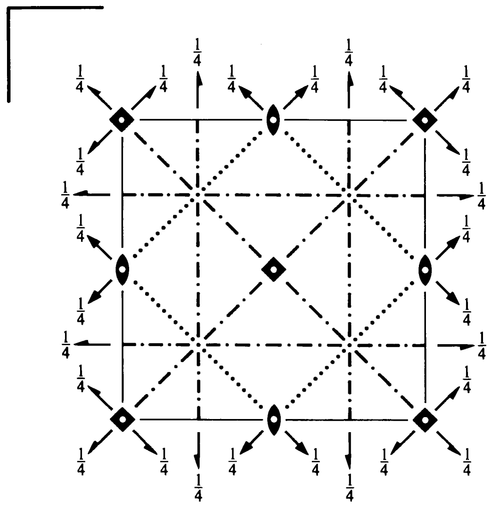
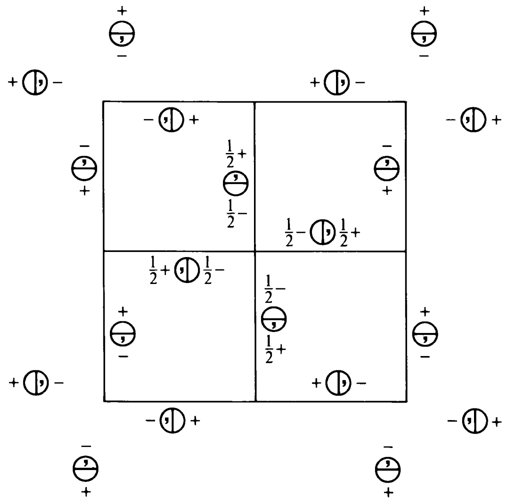
International Tables for Crystallography (2016). Vol. A, Space group 128, pp. 456–457.

$P4/mnc$ D_{4h}^{6} $4/mmm$ Tetragonal

No. 128 $P\ 4/m\ 2_1/n\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/m\,1\,n$

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

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^{+}\quad 0,0,z$	(4) $4^{-}\quad 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(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) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

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	i	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (10) $x,y,\bar{z}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	$m\,.\,.$	$x,y,0$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{y},0$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{y},x,0$ $y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y,\bar{x},0$ $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
8	g	$.\,.\,2$	$x,x+\frac{1}{2},\frac{1}{4}$ $\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x,x+\frac{1}{2},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$ $\bar{x}+\frac{1}{2},x,\frac{3}{4}$	hkl: $l=2n$
8	f	$2\,.\,.$	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$ $\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k,l=2n$
4	e	$4\,.\,.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	d	$2\,.\,22$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,l=2n$
2	b	$4/m\,.\,.$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$4/m\,.\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

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