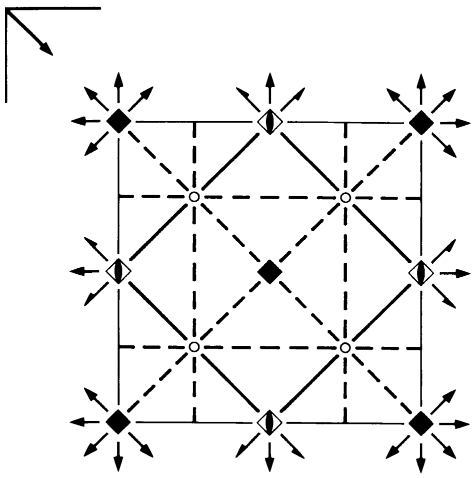
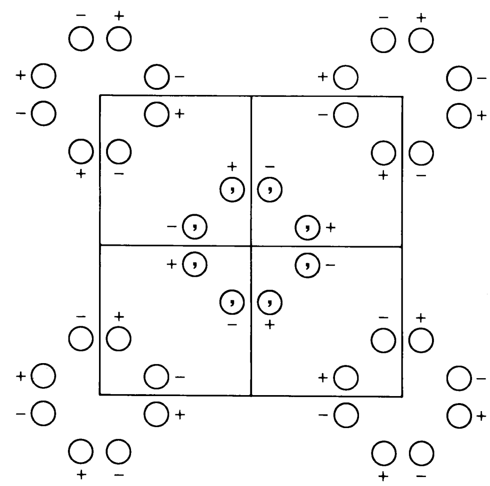
$P4/nbm$ D_{4h}^{3} $4/mmm$ Tetragonal

No. 125 $P\ 4/n\ 2/b\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at 422 at $4/n22/g$, at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

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

Symmetry operations

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

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	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	m	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x,\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x,\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	
8	l	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	k	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	
8	j	$..2$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	i	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	
4	h	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k=2n$
4	g	$4..$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hkl: $h,k=2n$
2	d	$\bar{4}2m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{4}2m$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	b	422	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	422	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

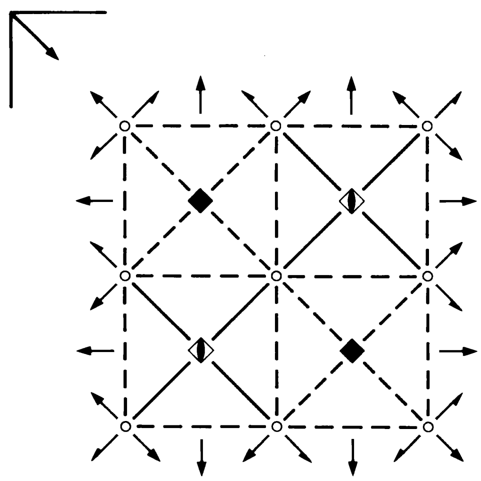
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

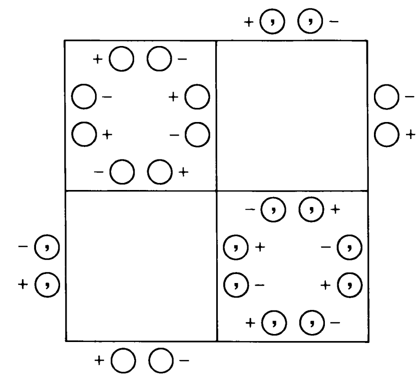
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4/nbm$ D_{4h}^{3} $4/mmm$ Tetragonal

No. 125 $P\ 4/n\ 2/b\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4},\frac{1}{4},0$ from 422

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

Symmetry operations

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

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	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	m	$..m$	$x,\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z$	$x+\frac{1}{2},x,z$	$\bar{x},\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},x,\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	l	$.2.$	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},x,\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\bar{x},\frac{1}{2}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{2}$	
8	k	$.2.$	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\frac{1}{4},x,0$	$\frac{1}{4},\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	$\frac{3}{4},\bar{x},0$	$\frac{3}{4},x+\frac{1}{2},0$	
8	j	$..2$	$x,x,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},\bar{x},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	
8	i	$..2$	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},\bar{x},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x},x+\frac{1}{2},0$	
4	h	$2.mm$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl: $h+k=2n$
4	g	$4..$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	hkl: $h+k=2n$
4	f	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	e	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	d	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{4}2m$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl: $h+k=2n$
2	b	422	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	a	422	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

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

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