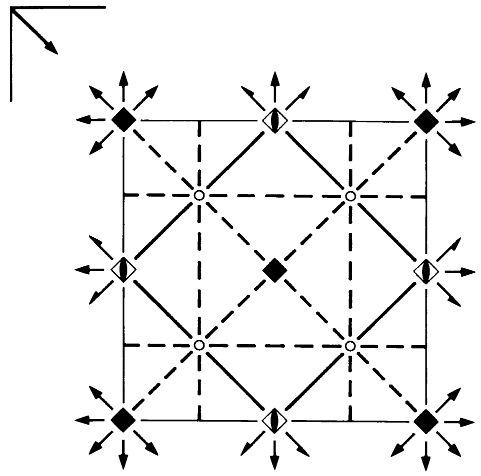
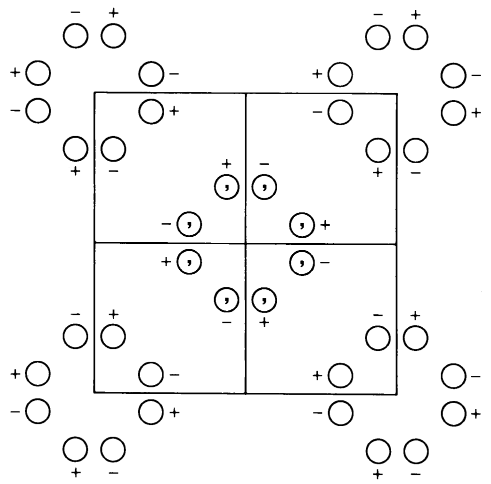
International Tables for Crystallography (2006). Vol. A, Space group 125, pp. 434–435.

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

No. 125 $\quad P\ 4/n\ 2/b\ 2/m$ $\quad$ 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 $\quad 0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le \frac{1}{2}-x$

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) $g(\frac{1}{2},\frac{1}{2},0)$ $\;x,x,z$

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [2] $P4/nbm$ ($\mathbf{c}'=2\mathbf{c}$) (125); [9] $P4/nbm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (125)

Minimal non-isomorphic supergroups

I $\quad$ none

II $\quad$ [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mcm$ (140)

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

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2/b1$ ($Pban$, 50)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/nnm$ ($\mathbf{c}'=2\mathbf{c}$) (134); [2] $P4_2/nbc$ ($\mathbf{c}'=2\mathbf{c}$) (133); [2] $P4/nnc$ ($\mathbf{c}'=2\mathbf{c}$) (126)

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