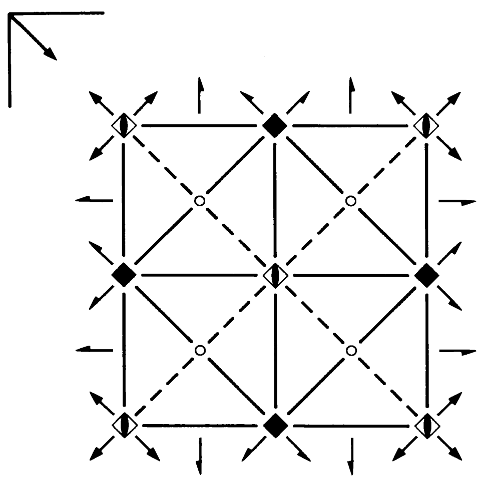
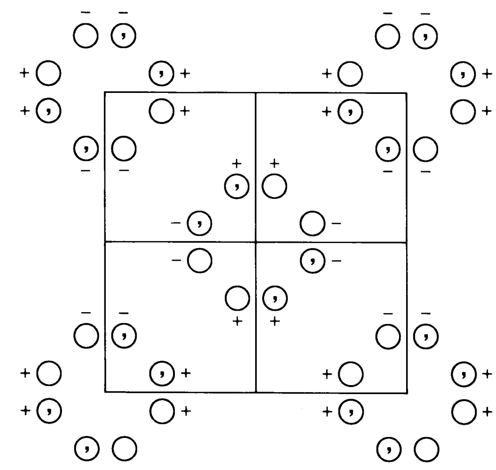
$P4/nmm$ D_{4h}^{7} $4/mmm$ Tetragonal

No. 129 $P\ 4/n\ 2_1/m\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, 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) $4^{+}\ \ 0,\frac{1}{2},z$	(4) $4^{-}\ \ \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$	(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) $\bar{4}^{+}\ \ 0,0,z;\ \ 0,0,0$	(12) $\bar{4}^{-}\ \ 0,0,z;\ \ 0,0,0$
(13) $m\ \ x,0,z$	(14) $m\ \ 0,y,z$	(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	k	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) $y+\frac{1}{2},x+\frac{1}{2},z$	$hk0$: $h+k=2n$ $h00$: $h=2n$
							Special: as above, plus
8	j	$..m$	$x,x+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},x,\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x},x+\frac{1}{2},z$ $x+\frac{1}{2},x,\bar{z}$	$x,\bar{x}+\frac{1}{2},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	no extra conditions
8	i	$.m.$	$0,y,z$ $\frac{1}{2},y+\frac{1}{2},\bar{z}$	$0,\bar{y},z$ $\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z$ $y,0,\bar{z}$	$y+\frac{1}{2},\frac{1}{2},z$ $\bar{y},0,\bar{z}$	no extra conditions
8	h	$..2$	$x,x,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x,\bar{x},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x,\frac{1}{2}$	hkl : $h+k=2n$
8	g	$..2$	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x},\bar{x},0$ $x+\frac{1}{2},x+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$ $x,\bar{x},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$ $\bar{x},x,0$	hkl : $h+k=2n$
4	f	$2mm.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl : $h+k=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl : $h,k=2n$
4	d	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl : $h,k=2n$
2	c	$4mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	b	$\bar{4}m2$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $h+k=2n$
2	a	$\bar{4}m2$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			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] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

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] $P\bar{4}m2$ (115) 1; 2; 7; 8; 11; 12; 13; 14
[2] $P\bar{4}2_1m$ (113) 1; 2; 5; 6; 11; 12; 15; 16
[2] $P4mm$ (99) 1; 2; 3; 4; 13; 14; 15; 16
[2] $P42_12$ (90) 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] $P2/n2_1/m1$ ($Pmmn$, 59) 1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $P4_2/ncm$ ($\mathbf{c}'=2\mathbf{c}$) (138); [2] $P4_2/nmc$ ($\mathbf{c}'=2\mathbf{c}$) (137); [2] $P4/ncc$ ($\mathbf{c}'=2\mathbf{c}$) (130)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}'=2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

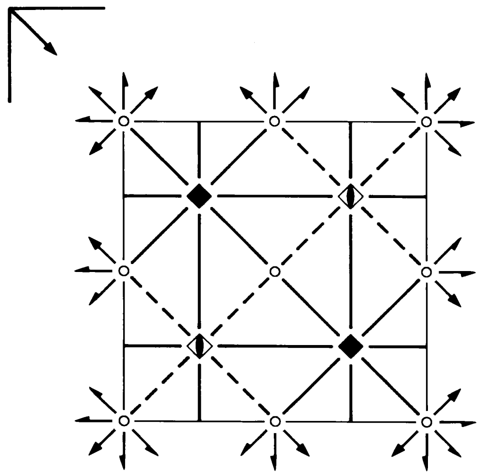
I none

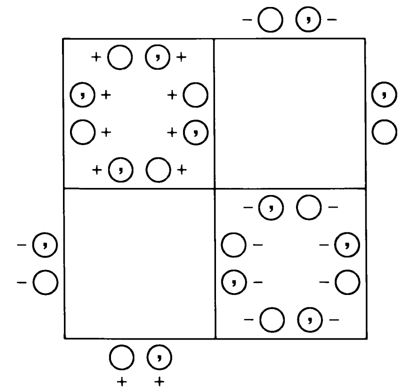
II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)

$P4/nmm$ D_{4h}^{7} $4/mmm$ Tetragonal

No. 129 $P\ 4/n\ 2_1/m\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n2_1$ $(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

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

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) $2(0,\frac{1}{2},0)\ \ 0,y,0$	(6) $2(\frac{1}{2},0,0)\ \ x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$
(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) $m\ \ x,\frac{1}{4},z$	(14) $m\ \ \frac{1}{4},y,z$	(15) $m\ \ x+\frac{1}{2},\bar{x},z$	(16) $m\ \ x,x,z$

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	k	1	(1) x,y,z (5) $\bar{x},y+\frac{1}{2},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y}+\frac{1}{2},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},\bar{y},\bar{z}$ (10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (14) $\bar{x}+\frac{1}{2},y,z$	(3) $\bar{y}+\frac{1}{2},x,z$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$ (11) $y+\frac{1}{2},\bar{x},\bar{z}$ (15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $y,\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x+\frac{1}{2},\bar{z}$ (16) y,x,z	$hk0: h+k=2n$ $h00: h=2n$
							Special: as above, plus
8	j	$..m$	x,x,z $\bar{x},x+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$ $x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,z$ $x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x,\bar{x}+\frac{1}{2},z$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	i	$.m.$	$\frac{1}{4},y,z$ $\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$ $\frac{3}{4},\bar{y},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{4},z$ $y+\frac{1}{2},\frac{3}{4},\bar{z}$	$y,\frac{1}{4},z$ $\bar{y},\frac{3}{4},\bar{z}$	no extra conditions
8	h	$..2$	$x,\bar{x},\frac{1}{2}$ $\bar{x},x,\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x,x+\frac{1}{2},\frac{1}{2}$	$hkl: h+k=2n$
8	g	$..2$	$x,\bar{x},0$ $\bar{x},x,0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x,0$ $\bar{x}+\frac{1}{2},\bar{x},0$	$\bar{x},\bar{x}+\frac{1}{2},0$ $x,x+\frac{1}{2},0$	$hkl: h+k=2n$
4	f	$2mm.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$hkl: h+k=2n$
4	e	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$hkl: h,k=2n$
4	d	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$hkl: h,k=2n$
2	c	$4mm$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			$hkl: h+k=2n$
2	a	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			$hkl: h+k=2n$

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

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

Maximal non-isomorphic subgroups

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Maximal isomorphic subgroups of lowest index

IIc [2] $P4/nmm$ ($\mathbf{c}'=2\mathbf{c}$) (129); [9] $P4/nmm$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (129)

Minimal non-isomorphic supergroups

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II [2] $C4/mmm$ ($P4/mmm$, 123); [2] $I4/mmm$ (139)