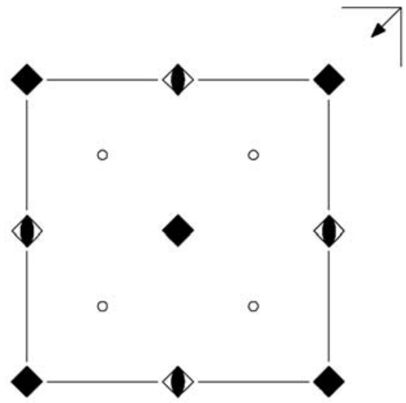
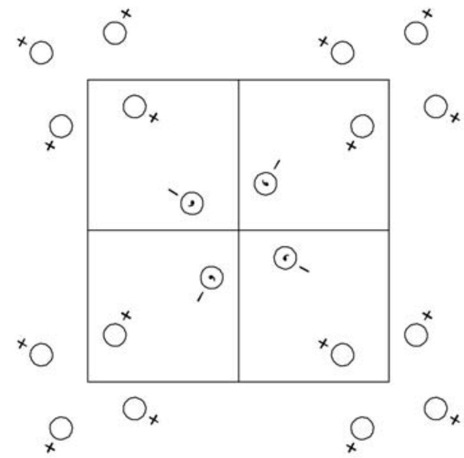
International Tables for Crystallography (2006). Vol. E, Layer group 52, pp. 326–329.

$p4/n$ $4/m$ Tetragonal/Square

No. 52 $p4/n$ Patterson symmetry $p4/m$

ORIGIN CHOICE 1





Origin at 4 on n at $-\frac{1}{4},-\frac{1}{4},0$ from $\bar{1}$

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

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y},x,z$ (7) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*d*	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4	*c*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hk: $h,k=2n$
2	*b*	4 . .	$\frac{1}{2},\frac{1}{2},z$	$0,0,\bar{z}$			no extra conditions
2	*a*	$\bar{4}$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,\frac{1}{4},0$

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

Maximal non-isotypic subgroups

I [2] $p\bar{4}$ (50) 1; 2; 7; 8
[2] $p4$ (49) 1; 2; 3; 4
[2] $p2/n11$ ($p112/a$, 7) 1; 2; 5; 6

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [5] $p4/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (52)

Minimal non-isotypic supergroups

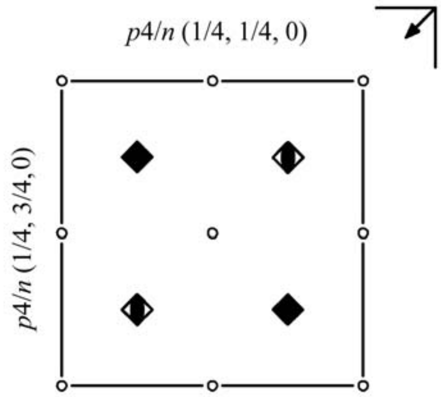
I [2] $p4/nbm$ (62); [2] $p4/nmm$ (64)

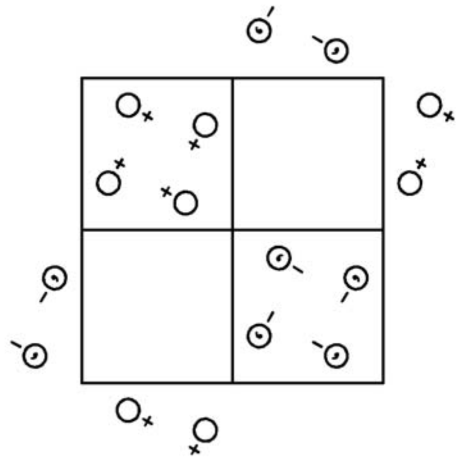
II [2] $c4/m$ ($p4/m$, 51)

$p4/n$ $(\frac{1}{4},\frac{1}{4},0)$ $4/m$ Tetragonal/Square

No. 52 $p4/n$ Patterson symmetry $p4/m$

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n at $\frac{1}{4},\frac{1}{4},0$ from 4

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

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) $\bar{1}$ 0,0,0	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$	(8) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x,z$ (7) $y+\frac{1}{2},\bar{x},\bar{z}$	(4) $y,\bar{x}+\frac{1}{2},z$ (8) $\bar{y},x+\frac{1}{2},\bar{z}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
							Special: as above, plus
4	*d*	$2\,.\,.$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	no extra conditions
4	*c*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	*b*	$4\,.\,.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	*a*	$\bar{4}\,.\,.$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $\not{p}2mg$
$\mathbf{a}'=\mathbf{b}$
Origin at $x,0,0$

Along [110] $\not{p}2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I	[2] $p\bar{4}$ (50)	1; 2; 7; 8
	[2] $p4$ (49)	1; 2; 3; 4
	[2] $p2/n11$ ($p112/a$, 7)	1; 2; 5; 6
IIa	none	
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [5] $p4/n$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b},\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) (52)

Minimal non-isotypic supergroups

I [2] $p4/nbm$ (62); [2] $p4/nmm$ (64)

II [2] $c4/m$ ($p4/m$, 51)