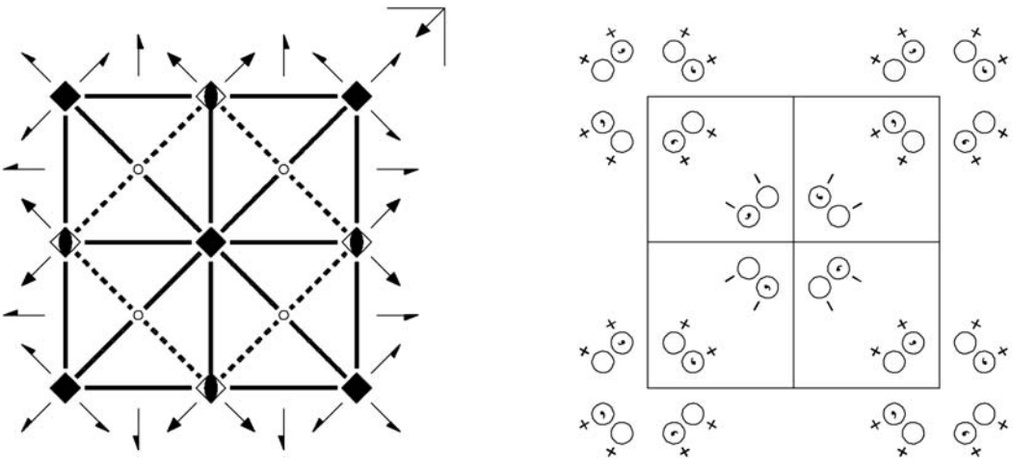
$p4/nmm$ $4/mmm$ Tetragonal/Square

No. 64 $p4/n2_1/m2/m$ Patterson symmetry $p4/mmm$

ORIGIN CHOICE 1



Origin on $4mm$ at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

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

Symmetry operations

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hk: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0k$: $k=2n$
			(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) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h0$: $h=2n$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	g	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	f	$.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z$	$y,0,z$	no extra conditions
			$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$y+\frac{1}{2},\frac{1}{2},\bar{z}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}$	
8	e	$..2$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},0$	$x+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	$\bar{x},x+\frac{1}{2},0$	
4	d	$2\,mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	no extra conditions
4	c	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hk: $h,k=2n$
2	b	$4\,m\,m$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	a	$\bar{4}\,m\,2$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			no extra conditions

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] $\not p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,\frac{1}{4},0$

Along [110] $\not p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$
Origin at $x,x,0$

Maximal non-isotypic subgroups

I	[2] $p\bar{4}m2$ (59)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $p\bar{4}2_1m$ (58)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4mm$ (55)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p42_12$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $p4/n11$ ($p4/n$, 52)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $p2/n12/m$ ($cmme$, 48)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $p2/n2_1/m1$ ($pmmn$, 46)	1; 2; 5; 6; 9; 10; 13; 14
IIa	none	
IIb	none	

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nmm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (64)

Minimal non-isotypic supergroups

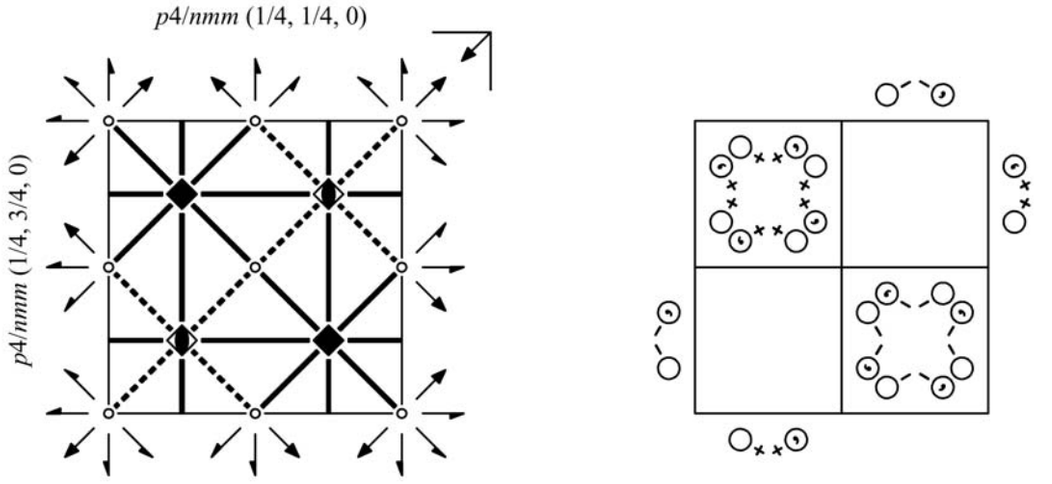
I none

II [2] $c4/mmm$ ($p4/mmm$, 61)

No. 64 $p4/n2_1/m2/m$

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 $4mm$

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

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) $2(0,\frac{1}{2},0)$ $0,y,0$	(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); $t(1,0,0)$; $t(0,1,0)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	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) $y,\bar{x}+\frac{1}{2},z$	hk: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0k$: $k=2n$
			(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) $\bar{y},x+\frac{1}{2},\bar{z}$	$h0$: $h=2n$
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z	
							Special: as above, plus
8	g	$..m$	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x,\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	f	$.m.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\bar{y}+\frac{1}{2},\frac{1}{4},z$	$y,\frac{1}{4},z$	no extra conditions
			$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	$y+\frac{1}{2},\frac{3}{4},\bar{z}$	$\bar{y},\frac{3}{4},\bar{z}$	
8	e	$..2$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},x,0$	$\bar{x},\bar{x}+\frac{1}{2},0$	no extra conditions
			$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x},0$	$x,x+\frac{1}{2},0$	
4	d	$2mm.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	no extra conditions
4	c	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hk: $h,k=2n$
2	b	$4mm$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	a	$\bar{4}m2$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			no extra conditions

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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] $\not p2mg$
$\mathbf{a}' = \mathbf{b}$
Origin at $x,0,0$

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

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