

$p4/nmm$

$4/mmm$

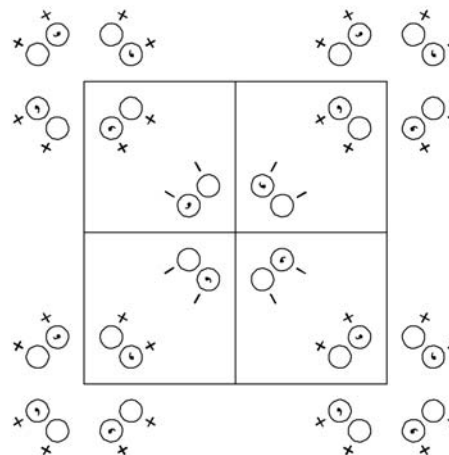
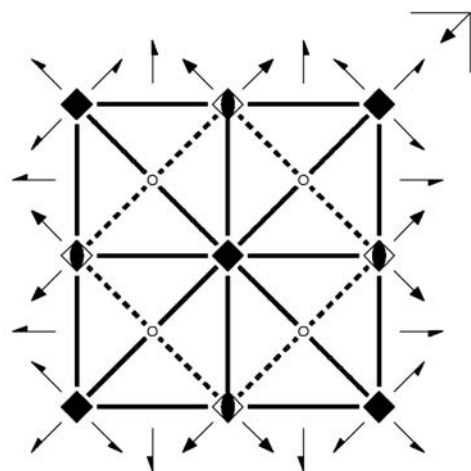
Tetragonal/Square

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 $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; y \leq \frac{1}{2} - x; 0 \leq z$

Symmetry operations

- | | | | |
|---|---|--|---|
| (1) 1
(1 0,0,0) | (2) 2 0,0,z
(2 _z 0,0,0) | (3) 4 ⁺ 0,0,z
(4 _z ⁺ 0,0,0) | (4) 4 ⁻ 0,0,z
(4 _z ⁻ 0,0,0) |
| (5) 2($\frac{1}{2}, \frac{1}{2}, 0$) 0,y,0
(2 _y \frac{1}{2}, \frac{1}{2}, 0) | (6) 2($\frac{1}{2}, \frac{1}{2}, 0$) x,0,0
(2 _x \frac{1}{2}, \frac{1}{2}, 0) | (7) 2($\frac{1}{2}, \frac{1}{2}, 0$) x,x,0
(2 _{xy} \frac{1}{2}, \frac{1}{2}, 0) | (8) 2($\frac{1}{2}, \frac{1}{2}, 0$) x, \bar{x} ,0
(2 _{$\bar{y}x$} \frac{1}{2}, \frac{1}{2}, 0) |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, 0$
($\bar{1}$ \frac{1}{2}, \frac{1}{2}, 0) | (10) n ($\frac{1}{2}, \frac{1}{2}, 0$) x,y,0
(m_z \frac{1}{2}, \frac{1}{2}, 0) | (11) $\bar{4}^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$
($\bar{4}_z^+$ \frac{1}{2}, \frac{1}{2}, 0) | (12) $\bar{4}^-$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$
($\bar{4}_z^-$ \frac{1}{2}, \frac{1}{2}, 0) |
| (13) m x,0,z
(m_y 0,0,0) | (14) m 0,y,z
(m_x 0,0,0) | (15) m x, \bar{x} ,z
(m_{xy} 0,0,0) | (16) m x,x,z
($m_{\bar{y}x}$ 0,0,0) |

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

Positions

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

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] $\neq 2mg$
 $\mathbf{a}' = \mathbf{b}$
 Origin at $x, \frac{1}{4}, 0$

Along [110] $\neq 2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$
 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] $p4_22$ (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)

$p4/nmm$ $(\frac{1}{4}, \frac{1}{4}, 0)$ $4/mmm$

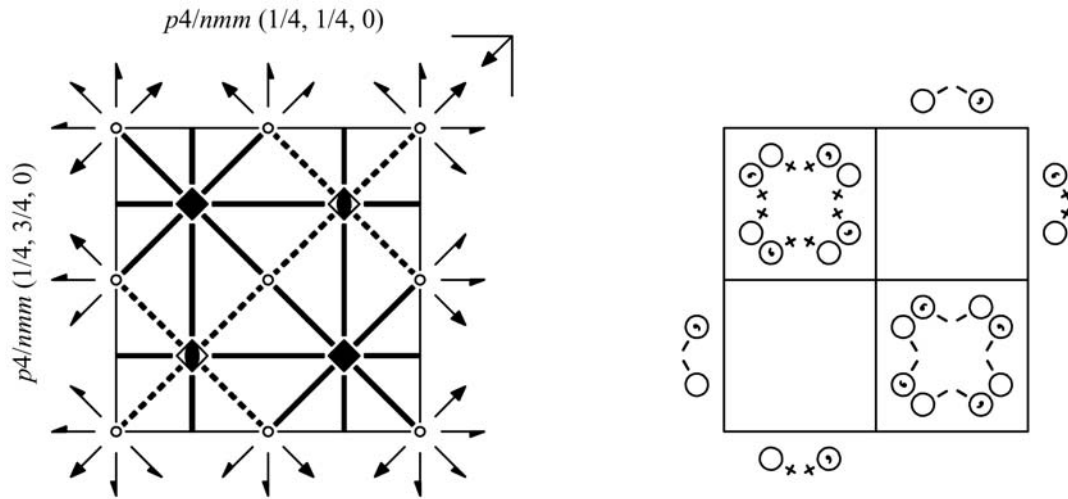
Tetragonal/Square

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

Symmetry operations

- | | | | |
|---|--|--|--|
| (1) 1
(1 0,0,0) | (2) $2_{\frac{1}{4}, \frac{1}{4}, z}$
($2_z \frac{1}{2}, \frac{1}{2}, 0$) | (3) $4^+_{\frac{1}{4}, \frac{1}{4}, z}$
($4_z \frac{1}{2}, 0, 0$) | (4) $4^-_{\frac{1}{4}, \frac{1}{4}, z}$
($4_z^{-1} 0, \frac{1}{2}, 0$) |
| (5) $2(0, \frac{1}{2}, 0)$ $0, y, 0$
($2_y 0, \frac{1}{2}, 0$) | (6) $2(\frac{1}{2}, 0, 0)$ $x, 0, 0$
($2_x \frac{1}{2}, 0, 0$) | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$
($2_{xy} \frac{1}{2}, \frac{1}{2}, 0$) | (8) 2 $x, \bar{x}, 0$
($2_{\bar{y}} 0, 0, 0$) |
| (9) $\bar{1}$ $0, 0, 0$
($\bar{1} 0, 0, 0$) | (10) $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$
($m_z \frac{1}{2}, \frac{1}{2}, 0$) | (11) $\bar{4}^+_{\frac{1}{4}, -\frac{1}{4}, z}; \frac{1}{4}, -\frac{1}{4}, 0$
($\bar{4}_z \frac{1}{2}, 0, 0$) | (12) $\bar{4}^-_{\frac{1}{4}, \frac{1}{4}, z}; -\frac{1}{4}, \frac{1}{4}, 0$
($\bar{4}_z^{-1} 0, \frac{1}{2}, 0$) |
| (13) m $x, \frac{1}{4}, z$
($m_y 0, \frac{1}{2}, 0$) | (14) m $\frac{1}{4}, y, z$
($m_x \frac{1}{2}, 0, 0$) | (15) m $x + \frac{1}{2}, \bar{x}, z$
($m_{xy} \frac{1}{2}, \frac{1}{2}, 0$) | (16) m x, x, z
($m_{\bar{y}} 0, 0, 0$) |

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
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				General:			
16	h	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	$hk: h + k = 2n$ $0k: k = 2n$ $h0: h = 2n$

Special: as above, plus

8	g	$. . m$	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	f	$. m .$	$\frac{1}{4}, y, z$ $\frac{3}{4}, y + \frac{1}{2}, \bar{z}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, z$ $\frac{3}{4}, \bar{y}, \bar{z}$	$\bar{y} + \frac{1}{4}, \frac{1}{4}, z$ $y + \frac{1}{2}, \frac{3}{4}, \bar{z}$	$y, \frac{1}{4}, z$ $\bar{y}, \frac{3}{4}, \bar{z}$	no extra conditions
8	e	$. . 2$	$x, \bar{x}, 0$ $\bar{x}, x, 0$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x + \frac{1}{2}, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$ $x, x + \frac{1}{2}, 0$	no extra conditions
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	$4m m$	$\frac{1}{4}, \frac{1}{4}, z$	$\frac{3}{4}, \frac{3}{4}, \bar{z}$			no extra conditions
2	a	$\bar{4}m 2$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$			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 $\frac{1}{4}, \frac{1}{4}, z$

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

Along [110] $\not\neq 2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$
 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] $p\bar{4}2, m$ (58)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4mm$ (55)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p42, 2$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $p4/n 11$ ($p4/n, 52$)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $p2/n 12/m$ ($cmme, 48$)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $p2/n 2_1/m 1$ ($pmmn, 46$)	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] $c4/mmm$ ($p4/mmm, 61$)