

$p4/nbm$

$4/mmm$

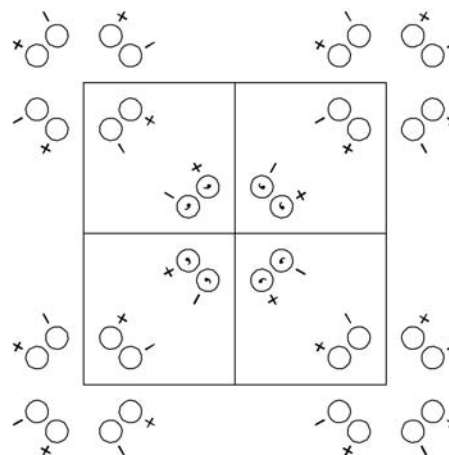
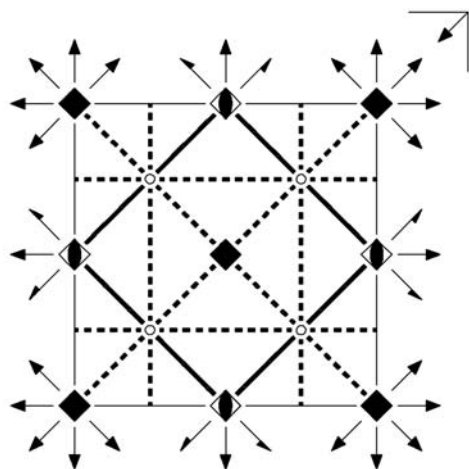
Tetragonal/Square

No. 62

$p4/n2/b2/m$

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

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (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) $\bar{4}^-$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, 0$ |
| (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 |

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>i</i> 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) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk: h + k = 2n$ $0k: k = 2n$ $h0: h = 2n$ Special: as above, plus
8	<i>h</i> . . <i>m</i>	$x, x + \frac{1}{2}, z$ $\bar{x}, x + \frac{1}{2}, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, z$ $x + \frac{1}{2}, x, \bar{z}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$	no extra conditions
8	<i>g</i> . 2 .	$x, 0, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$	$\bar{x}, 0, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$	$0, x, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$0, \bar{x}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$	no extra conditions
8	<i>f</i> . . 2	$x, x, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$	$\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	$x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	no extra conditions
4	<i>e</i> 2 . <i>mm</i>	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	no extra conditions
4	<i>d</i> 4 . .	$0, 0, z$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	no extra conditions
4	<i>c</i> . . 2/ <i>m</i>	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$\frac{1}{4}, \frac{3}{4}, 0$	$hk: h, k = 2n$
2	<i>b</i> $\bar{4} 2 m$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			no extra conditions
2	<i>a</i> 4 2 2	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			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] $\bar{4} 2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
 Origin at $x, 0, 0$

Along [110] $\bar{4} 2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$
 Origin at $x, x, 0$

Maximal non-isotypic subgroups

I	[2] $p\bar{4}b2$ (60)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $p\bar{4}2m$ (57)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4bm$ (56)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p422$ (53)	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] $p2/n2/b1$ ($pban$, 39)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/nbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (62)

Minimal non-isotypic supergroups

I none

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

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

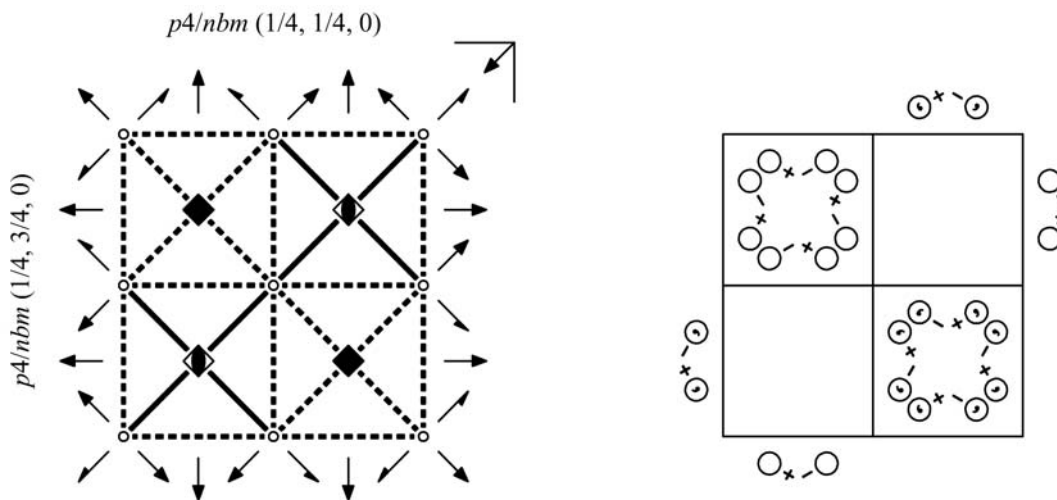
Tetragonal/Square

No. 62

$p4/n2/b2/m$

Patterson symmetry $p4/mmm$

ORIGIN CHOICE 2



Origin at centre ($2/m$) at $n(\mathbf{b}, \mathbf{a})(2_1/g, 2/m)$ at $\frac{1}{4}, \frac{1}{4}, 0$ from 422

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
16 <i>i</i> 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) $y, \bar{x} + \frac{1}{2}, z$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z}$ (7) y, x, \bar{z} (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (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) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$ (14) $\bar{x}, y + \frac{1}{2}, z$ (15) \bar{y}, \bar{x}, z (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk: h + k = 2n$ $0k: k = 2n$ $h0: h = 2n$ Special: as above, plus
8 <i>h</i> $\dots m$	x, \bar{x}, z $\bar{x} + \frac{1}{2}, \bar{x}, \bar{z}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z$ $x, x + \frac{1}{2}, \bar{z}$ $x + \frac{1}{2}, x, z$ \bar{x}, x, \bar{z} $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8 <i>g</i> \dots	$x, \frac{1}{4}, 0$ $\bar{x}, \frac{3}{4}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, 0$ $x + \frac{1}{2}, \frac{3}{4}, 0$ $\frac{1}{4}, x, 0$ $\frac{3}{4}, \bar{x}, 0$ $\frac{1}{4}, \bar{x} + \frac{1}{2}, 0$ $\frac{3}{4}, x + \frac{1}{2}, 0$	no extra conditions
8 <i>f</i> $\dots 2$	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$ $x, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x + \frac{1}{2}, 0$	no extra conditions
4 <i>e</i> $2 \dots mm$	$\frac{3}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{3}{4}, z$ $\frac{3}{4}, \frac{1}{4}, \bar{z}$ $\frac{1}{4}, \frac{3}{4}, \bar{z}$	no extra conditions
4 <i>d</i> $4 \dots$	$\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, \bar{z}$ $\frac{3}{4}, \frac{3}{4}, z$	no extra conditions
4 <i>c</i> $\dots 2/m$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, 0$	$hk: h, k = 2n$
2 <i>b</i> $\bar{4} 2 m$	$\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$	no extra conditions
2 <i>a</i> $4 2 2$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$	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 $[100] \bar{4} 2 mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
 Origin at $x, 0, 0$

Along $[110] \bar{4} 2 mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$
 Origin at $x, x, 0$

Maximal non-isotypic subgroups

I	$[2] p\bar{4}b2$ (60)	1; 2; 7; 8; 11; 12; 13; 14
	$[2] p\bar{4}2m$ (57)	1; 2; 5; 6; 11; 12; 15; 16
	$[2] p4bm$ (56)	1; 2; 3; 4; 13; 14; 15; 16
	$[2] p422$ (53)	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
	$[2] p2/n 2/b 1$ ($pban$, 39)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc $[9] p4/nbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (62)

Minimal non-isotypic supergroups

I none

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