

$p4/nbm$

$4/mmm$

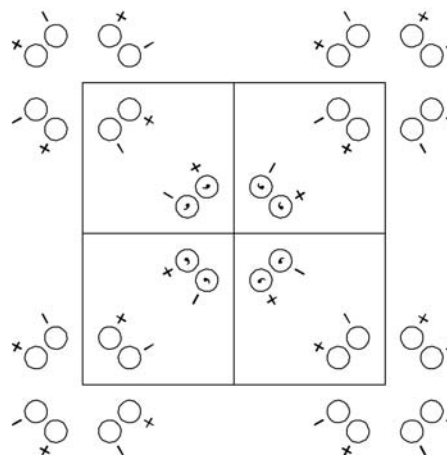
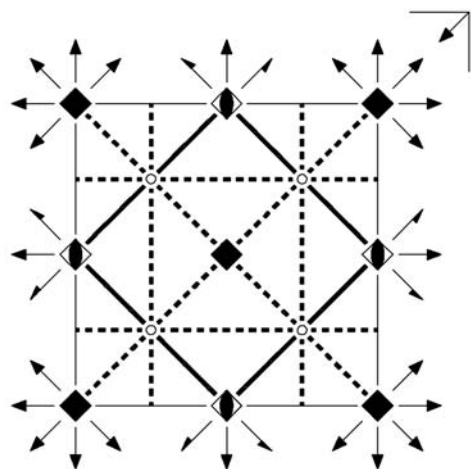
Tetragonal/Square

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
(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 0,y,0
(2 _y 0,0,0) | (6) 2 x,0,0
(2 _x 0,0,0) | (7) 2 x,x,0
(2 _{xy} 0,0,0) | (8) 2 x,x̄,0
(2 _{xȳ} 0,0,0) |
| (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) a x, $\frac{1}{4}, z$
(m_y $\frac{1}{2}, \frac{1}{2}, 0$) | (14) b $\frac{1}{4}, y, z$
(m_x $\frac{1}{2}, \frac{1}{2}, 0$) | (15) m x + $\frac{1}{2}, \bar{x}, z$
(m_{xy} $\frac{1}{2}, \frac{1}{2}, 0$) | (16) g($\frac{1}{2}, \frac{1}{2}, 0$) x,x,z
(m_{xy} $\frac{1}{2}, \frac{1}{2}, 0$) |

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>i</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) y, x, z (4) y, \bar{x}, z (5) \bar{x}, y, \bar{z} (6) x, \bar{y}, \bar{z} (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ (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) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$ (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $hk: h+k=2n$ $0k: k=2n$ $h0: h=2n$
8 <i>h</i> $\dots m$	$x, x + \frac{1}{2}, z$ $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x, \bar{x} + \frac{1}{2}, \bar{z}$ $\bar{x}, \bar{x} + \frac{1}{2}, \bar{z}$	Special: as above, plus no extra conditions
8 <i>g</i> $\dots 2$	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, 0$ $0, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, \frac{1}{2}, 0$ $x + \frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\frac{1}{2}, x + \frac{1}{2}, 0$	no extra conditions
8 <i>f</i> $\dots 2$	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $\bar{x}, x, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ $x, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$	no extra conditions
4 <i>e</i> $2 \dots mm$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $0, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, \bar{z}$	no extra conditions
4 <i>d</i> $4 \dots$	$0, 0, z$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$	no extra conditions
4 <i>c</i> $\dots 2/m$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{3}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$ $\frac{1}{4}, \frac{3}{4}, 0$	$hk: h, k = 2n$
2 <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 $[100] \not{p}2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
 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	$[2] p\bar{4}b2$ (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)

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

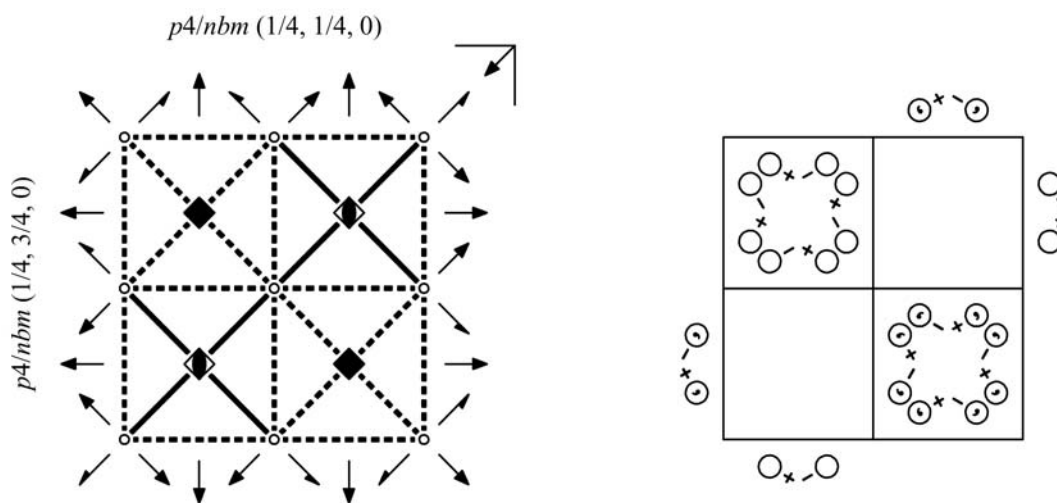
Tetragonal/Square

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

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>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: $hk: h+k=2n$ $0k: k=2n$ $h0: h=2n$
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} $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	Special: as above, plus 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
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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

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