

$p4/mbm$

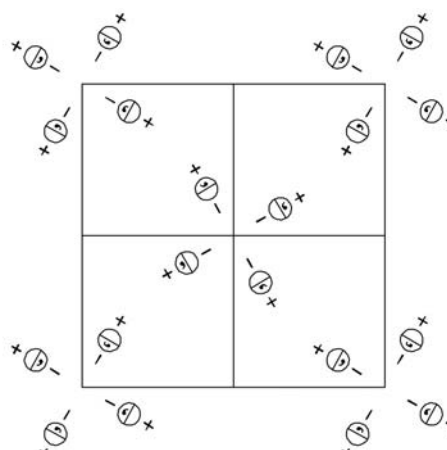
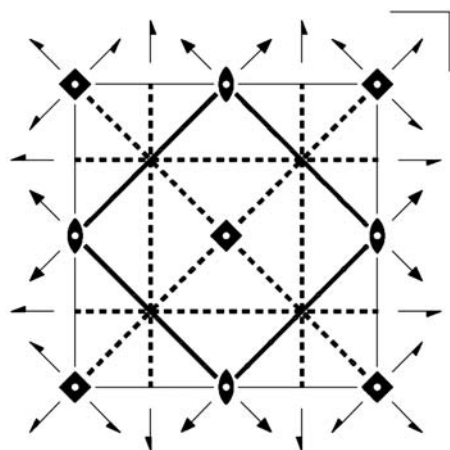
$4/mmm$

Tetragonal/Square

No. 63

$p4/m2_1/b2/m$

Patterson symmetry $p4/mmm$



Origin at centre ($4/m$) at $4/m12_1/g$

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) $2(0, \frac{1}{2}, 0) \ \frac{1}{4}, y, 0$ | (6) $2(\frac{1}{2}, 0, 0) \ x, \frac{1}{4}, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \ x, x, 0$ | (8) $2 \ x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1} \ 0,0,0$ | (10) $m \ x,y,0$ | (11) $\bar{4}^+ \ 0,0,z; 0,0,0$ | (12) $\bar{4}^- \ 0,0,z; 0,0,0$ |
| (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	h 1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ (10) x, y, \bar{z} (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	(3) \bar{y}, x, z (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) y, \bar{x}, \bar{z} (15) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(4) y, \bar{x}, z (8) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) $y + \frac{1}{2}, x + \frac{1}{2}, z$	General: $h0: h = 2n$ $0k: k = 2n$ Special: as above, plus
8	g $\dots m$	$x, x + \frac{1}{2}, z$ $\bar{x} + \frac{1}{2}, x, \bar{z}$	$\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, \bar{x}, \bar{z}$	$\bar{x} + \frac{1}{2}, x, z$ $x, x + \frac{1}{2}, \bar{z}$	$x + \frac{1}{2}, \bar{x}, z$ $\bar{x}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8	f $m \dots$	$x, y, 0$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, 0$	$\bar{x}, \bar{y}, 0$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	$\bar{y}, x, 0$ $y + \frac{1}{2}, x + \frac{1}{2}, 0$	$y, \bar{x}, 0$ $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$	no extra conditions
4	e $m \cdot 2m$	$x, x + \frac{1}{2}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, 0$	$x + \frac{1}{2}, \bar{x}, 0$	no extra conditions
4	d $2 \cdot mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$\frac{1}{2}, 0, \bar{z}$	$0, \frac{1}{2}, \bar{z}$	$hk: h + k = 2n$
4	c $4 \dots$	$0, 0, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$0, 0, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, z$	$hk: h + k = 2n$
2	b $m \cdot mm$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hk: h + k = 2n$
2	a $4/m \dots$	$0, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$			$hk: h + k = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $\not\sim 2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$
Origin at $x, 0, 0$

Along [110] $\not\sim 2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$
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] $p\bar{4}2_1m$ (58)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4bm$ (56)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p4_22$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $p4/m11$ ($p4/m$, 51)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $p2/m12/m$ ($cmmm$, 47)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $p2/m2_1/b1$ ($pbam$, 44)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isotypic subgroups of lowest index

IIc [9] $p4/mbm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (63)

Minimal non-isotypic supergroups

I none

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