

$p4/mbm$

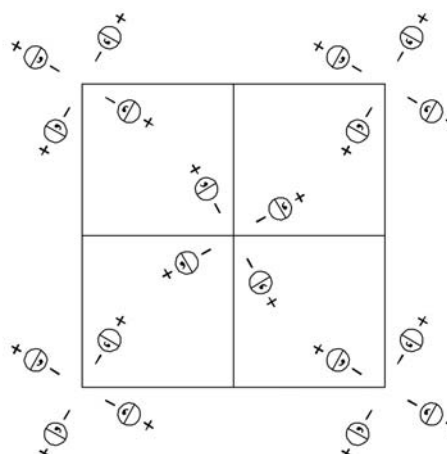
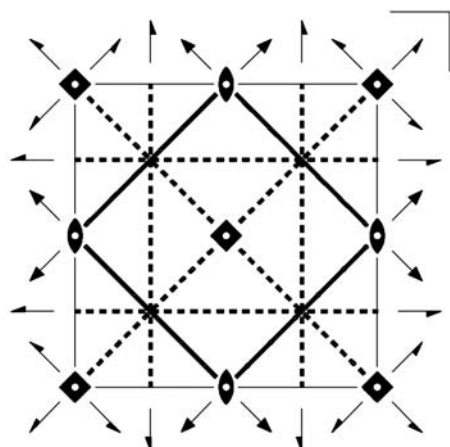
$4/mmm$

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
(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, $\frac{1}{2}$, 0) $\frac{1}{4}$, y, 0
(2 _y $\frac{1}{2}$, $\frac{1}{2}$, 0) | (6) 2($\frac{1}{2}$, 0, 0) x, $\frac{1}{4}$, 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 x, $\bar{x} + \frac{1}{2}$, 0
(2 _{\bar{xy}} $\frac{1}{2}$, $\frac{1}{2}$, 0) |
| (9) $\bar{1}$ 0,0,0
($\bar{1}$ 0,0,0) | (10) m x,y,0
(m _z 0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0
($\bar{4}_z^+$ 0,0,0) | (12) $\bar{4}^-$ 0,0,z; 0,0,0
($\bar{4}_z^-$ 0,0,0) |
| (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 _{\bar{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>h</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) \bar{y}, x, z (4) y, \bar{x}, z (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) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) y, \bar{x}, \bar{z} (12) \bar{y}, x, \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: $h0: h = 2n$ $0k: k = 2n$ Special: as above, plus
8 <i>g</i> $\dots m$	$x, x + \frac{1}{2}, z$ $\bar{x}, \bar{x} + \frac{1}{2}, z$ $x + \frac{1}{2}, x, \bar{z}$ $\bar{x}, \bar{x} + \frac{1}{2}, \bar{z}$	no extra conditions
8 <i>f</i> $m \dots$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $x + \frac{1}{2}, y + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, 0$	no extra conditions
4 <i>e</i> $m \cdot 2m$	$x, x + \frac{1}{2}, 0$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$ $\bar{x} + \frac{1}{2}, x, 0$ $x + \frac{1}{2}, \bar{x}, 0$	no extra conditions
4 <i>d</i> $2 \cdot mm$	$0, \frac{1}{2}, z$ $\frac{1}{2}, 0, z$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$	$hk: h + k = 2n$
4 <i>c</i> $4 \dots$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $0, 0, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, z$	$hk: h + k = 2n$
2 <i>b</i> $m \cdot mm$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, 0$	$hk: h + k = 2n$
2 <i>a</i> $4/m \dots$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$hk: h + k = 2n$

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)