

$p4/mmm$

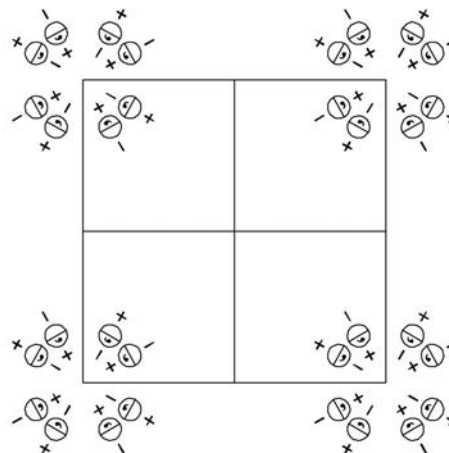
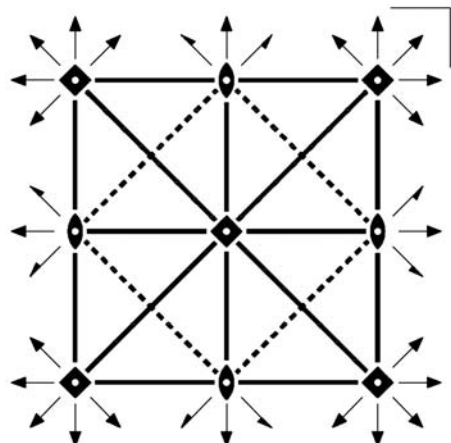
$4/mmm$

Tetragonal/Square

No. 61

$p4/m2/m2/m$

Patterson symmetry $p4/mmm$



Origin at centre ($4/mmm$)

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

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) $\bar{1}$ $0,0,0$ | (10) m $x,y,0$ | (11) $\bar{4}^+$ $0,0,z; 0,0,0$ | (12) $\bar{4}^-$ $0,0,z; 0,0,0$ |
| (13) m $x,0,z$ | (14) m $0,y,z$ | (15) m x,\bar{x},z | (16) m 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 n 1	(1) x, y, z (5) \bar{x}, y, \bar{z} (9) $\bar{x}, \bar{y}, \bar{z}$ (13) x, \bar{y}, z	(2) \bar{x}, \bar{y}, z (6) x, \bar{y}, \bar{z} (10) x, y, \bar{z} (14) \bar{x}, y, z	(3) \bar{y}, x, z (7) y, x, \bar{z} (11) y, \bar{x}, \bar{z} (15) \bar{y}, \bar{x}, z	(4) y, \bar{x}, z (8) $\bar{y}, \bar{x}, \bar{z}$ (12) \bar{y}, x, \bar{z} (16) y, x, z	General: no conditions	
8 m . m .	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	Special: no extra conditions	
8 l . m .	$x, 0, z$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z$ $x, 0, \bar{z}$	$0, x, z$ $0, x, \bar{z}$	$0, \bar{x}, z$ $0, \bar{x}, \bar{z}$	no extra conditions	
8 k . $.m$	x, x, z \bar{x}, x, \bar{z}	\bar{x}, \bar{x}, z x, \bar{x}, \bar{z}	\bar{x}, x, z x, x, \bar{z}	x, \bar{x}, z $\bar{x}, \bar{x}, \bar{z}$	no extra conditions	
8 j m . $.$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions	
4 i $m2m$.	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions	
4 h $m2m$.	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions	
4 g m . $2m$	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions	
4 f $2mm$.	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hk: h+k=2n$	
2 e $4mm$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions	
2 d $4mm$	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions	
2 c mmm .	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hk: h+k=2n$	
1 b $4/mmm$	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions	
1 a $4/mmm$	$0, 0, 0$				no extra conditions	

Symmetry of special projections

Along [001] $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, 0, z$

Along [100] $\not{p}2mm$
 $\mathbf{a}' = \mathbf{b}$
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] $p\bar{4}m2$ (59)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $p\bar{4}2m$ (57)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $p4mm$ (55)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $p422$ (53)	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] $p2/m2/m1$ ($pmmm$, 37)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb [2] $c4/amm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/nmm$, 64); [2] $c4/mmd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/mbm$, 63);
[2] $c4/amd$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/nbm$, 62)

Maximal isotypic subgroups of lowest index

IIc [2] $c4/mmm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($p4/mmm$, 61)

Minimal non-isotypic supergroups**I** none**II** none