

$p4/mmm$

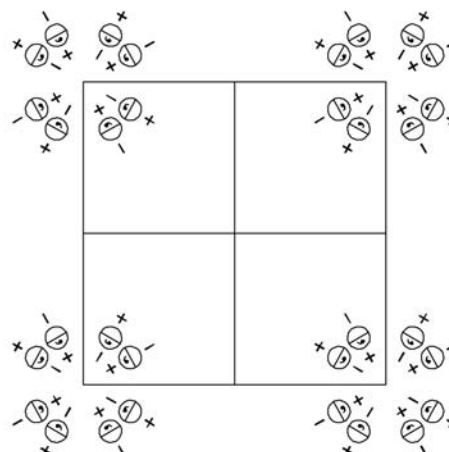
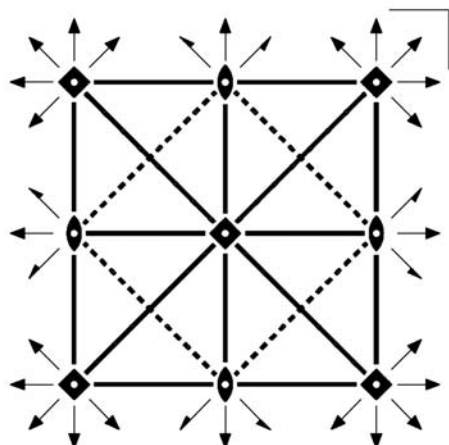
$4/mmm$

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<br>(1 0,0,0)                         | (2) 2 0,0,z<br>(2 <sub>z</sub>  0,0,0)  | (3) 4 <sup>+</sup> 0,0,z<br>(4 <sub>z</sub> <sup>+</sup>  0,0,0) | (4) 4 <sup>-</sup> 0,0,z<br>(4 <sub>z</sub> <sup>-</sup>  0,0,0) |
| (5) 2 0,y,0<br>(2 <sub>y</sub>  0,0,0)     | (6) 2 x,0,0<br>(2 <sub>x</sub>  0,0,0)  | (7) 2 x,x,0<br>(2 <sub>xy</sub>  0,0,0)                          | (8) 2 x,x̄,0<br>(2 <sub>xy</sub> <sup>-</sup>  0,0,0)            |
| (9) $\bar{1}$ 0,0,0<br>( $\bar{1}$  0,0,0) | (10) m x,y,0<br>(m <sub>z</sub>  0,0,0) | (11) $\bar{4}^+$ 0,0,z; 0,0,0<br>( $\bar{4}_z^+$  0,0,0)         | (12) $\bar{4}^-$ 0,0,z; 0,0,0<br>( $\bar{4}_z^-$  0,0,0)         |
| (13) m x,0,z<br>(m <sub>y</sub>  0,0,0)    | (14) m 0,y,z<br>(m <sub>x</sub>  0,0,0) | (15) m x,x̄,z<br>(m <sub>xy</sub>  0,0,0)                        | (16) m x,x,z<br>(m <sub>xy</sub> <sup>-</sup>  0,0,0)            |

**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	$n$	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  Special: no extra conditions
8	$m$	$.m.$	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	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  $[100] \not p2mm$   
 $\mathbf{a}' = \mathbf{b}$   
 Origin at  $x, 0, 0$

Along  $[110] \not p2mm$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$   
 Origin at  $x, x, 0$

**Maximal non-isotypic subgroups**

<b>I</b>	[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