

$P4_2/mnm$

D_{4h}^{14}

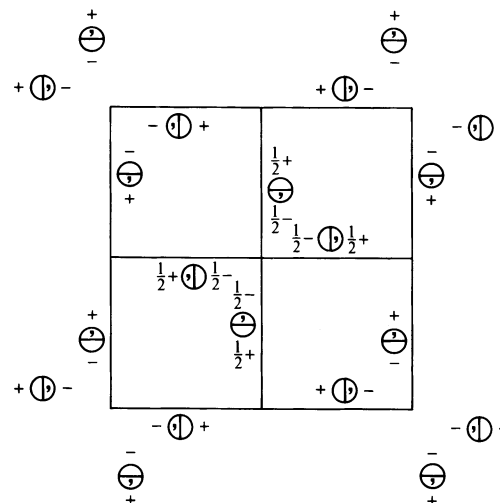
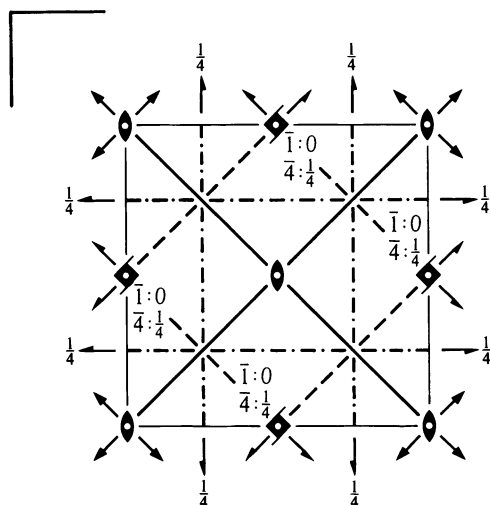
$4/mmm$

Tetragonal

No. 136

$P 4_2/m 2_1/n 2/m$

Patterson symmetry $P4/mmm$



Origin at centre (mmm) at $2/m12/m$

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

Symmetry operations

- | | | | |
|---|---|---|---|
| (1) 1 | (2) $2 \ 0,0,z$ | (3) $4^+(0,0,\frac{1}{2}) \ 0,\frac{1}{2},z$ | (4) $4^-(0,0,\frac{1}{2}) \ \frac{1}{2},0,z$ |
| (5) $2(0,\frac{1}{2},0) \ \frac{1}{4},y,\frac{1}{4}$ | (6) $2(\frac{1}{2},0,0) \ x,\frac{1}{4},\frac{1}{4}$ | (7) $2 \ x,x,0$ | (8) $2 \ x,\bar{x},0$ |
| (9) $\bar{1} \ 0,0,0$ | (10) $m \ x,y,0$ | (11) $\bar{4}^+ \ \frac{1}{2},0,z; \ \frac{1}{2},0,\frac{1}{4}$ | (12) $\bar{4}^- \ 0,\frac{1}{2},z; \ 0,\frac{1}{2},\frac{1}{4}$ |
| (13) $n(\frac{1}{2},0,\frac{1}{2}) \ x,\frac{1}{4},z$ | (14) $n(0,\frac{1}{2},\frac{1}{2}) \ \frac{1}{4},y,z$ | (15) $m \ x,\bar{x},z$ | (16) $m \ x,x,z$ |

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
16 <i>k</i> 1	(1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) x, y, \bar{z} (11) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (14) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (15) \bar{y}, \bar{x}, z (16) y, x, z	$0kl : k + l = 2n$ $00l : l = 2n$ $h00 : h = 2n$
		Special: as above, plus
8 <i>j</i> $\dots m$	x, x, z \bar{x}, \bar{x}, z $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ x, x, \bar{z} $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8 <i>i</i> $m \dots$	$x, y, 0$ $\bar{x}, \bar{y}, 0$ $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{2}$ $y, x, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
8 <i>h</i> $2 \dots$	$0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ $0, \frac{1}{2}, \bar{z}$ $0, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, z + \frac{1}{2}$ $\frac{1}{2}, 0, z$	$hkl : h + k, l = 2n$
4 <i>g</i> $m \cdot 2m$	$x, \bar{x}, 0$ $\bar{x}, x, 0$ $x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>f</i> $m \cdot 2m$	$x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$	no extra conditions
4 <i>e</i> $2 \cdot mm$	$0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$	$hkl : h + k + l = 2n$
4 <i>d</i> $\bar{4} \dots$	$0, \frac{1}{2}, \frac{1}{4}$ $0, \frac{1}{2}, \frac{3}{4}$ $\frac{1}{2}, 0, \frac{1}{4}$ $\frac{1}{2}, 0, \frac{3}{4}$	$hkl : h + k, l = 2n$
4 <i>c</i> $2/m \dots$	$0, \frac{1}{2}, 0$ $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, 0, 0$	$hkl : h + k, l = 2n$
2 <i>b</i> $m \cdot mm$	$0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h + k + l = 2n$
2 <i>a</i> $m \cdot mm$	$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : h + k + l = 2n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

Along [100] $c2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, 0, 0$

Along [110] $p2mm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I	[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}_2m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P4_22_2$ (94)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4_2/m11$ ($P4_2/m$, 84)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/m12/m$ ($Cmmm$, 65)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/m2_1/n1$ ($Pnmm$, 58)	1; 2; 5; 6; 9; 10; 13; 14

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_2/mnm$ ($\mathbf{c}' = 3\mathbf{c}$) (136); [9] $P4_2/mnm$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (136)

Minimal non-isomorphic supergroups

I none

II [2] $C4_2/mcm$ ($P4_2/mmc$, 131); [2] $I4/mmm$ (139); [2] $P4/mbm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (127)