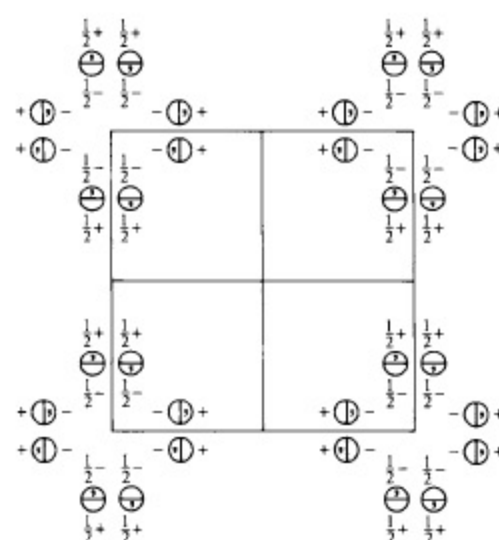
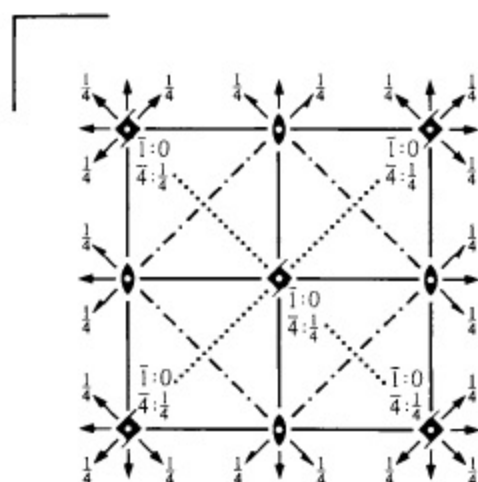


$P4_2/mmc$
 D_{4h}^9
 $4/mmm$

Tetragonal

No. 131

 $P 4_2/m 2/m 2/c$

Patterson symmetry $P4/mmm$

Origin at centre (mmm) at $4_2/m2/mc$
Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}$
Symmetry operations

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

Maximal non-isomorphic subgroups

- I**
- | | |
|---------------------------------|----------------------------|
| [2] $P\bar{4}m2$ (115) | 1; 2; 7; 8; 11; 12; 13; 14 |
| [2] $P\bar{4}2c$ (112) | 1; 2; 5; 6; 11; 12; 15; 16 |
| [2] $P4_2mc$ (105) | 1; 2; 3; 4; 13; 14; 15; 16 |
| [2] $P4_222$ (93) | 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] $P2/m12/c$ ($Cccm$, 66) | 1; 2; 7; 8; 9; 10; 15; 16 |
| [2] $P2/m2/m1$ ($Pmmm$, 47) | 1; 2; 5; 6; 9; 10; 13; 14 |

IIa none

- IIb**
- | |
|---|
| [2] $C4_2/emc$ ($a' = 2a, b' = 2b$) ($P4_2/ncm$, 138); [2] $C4_2/mmd$ ($a' = 2a, b' = 2b$) ($P4_2/mnm$, 136); |
| [2] $C4_2/emd$ ($a' = 2a, b' = 2b$) ($P4_2/nnm$, 134); [2] $C4_2/mmc$ ($a' = 2a, b' = 2b$) ($P4_2/mcm$, 132) |

Maximal isomorphic subgroups of lowest index

- IIc** [3] $P4_2/mmc$ ($c' = 3c$) (131); [9] $P4_2/mmc$ ($a' = 3a, b' = 3b$) (131)

Minimal non-isomorphic supergroups

- I** [3] $Pm\bar{3}n$ (223)
- II** [2] $C4_2/mmc$ ($P4_2/mcm$, 132); [2] $I4/mmm$ (139); [2] $P4/mmm$ ($c' = \frac{1}{2}c$) (123)

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	r 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) $\bar{y}, x, z + \frac{1}{2}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	$hhl : l = 2n$ $00l : l = 2n$
						Special: as above, plus
8	q $m..$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	p $.m.$	$\frac{1}{2}, y, z$ $\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, z$ $\frac{1}{2}, \bar{y}, \bar{z}$	$\bar{y}, \frac{1}{2}, z + \frac{1}{2}$ $y, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$y, \frac{1}{2}, z + \frac{1}{2}$ $\bar{y}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8	o $.m.$	$0, y, z$ $0, y, \bar{z}$	$0, \bar{y}, z$ $0, \bar{y}, \bar{z}$	$\bar{y}, 0, z + \frac{1}{2}$ $y, 0, \bar{z} + \frac{1}{2}$	$y, 0, z + \frac{1}{2}$ $\bar{y}, 0, \bar{z} + \frac{1}{2}$	no extra conditions
8	n $..2$	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{3}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$ $x, x, \frac{3}{2}$	$\bar{x}, x, \frac{3}{2}$ $x, \bar{x}, \frac{1}{2}$	$x, \bar{x}, \frac{3}{2}$ $\bar{x}, x, \frac{1}{2}$	$hkl : l = 2n$
4	m $m2m.$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	l $m2m.$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	k $m2m.$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	j $m2m.$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	i $2mm.$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z + \frac{1}{2}$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$	$hkl : h + k + l = 2n$
4	h $2mm.$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4	g $2mm.$	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
2	f $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$			$hkl : l = 2n$
2	e $\bar{4}m2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$			$hkl : l = 2n$
2	d $mmm.$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, 0$			$hkl : h + k + l = 2n$
2	c $mmm.$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl : h + k + l = 2n$
2	b $mmm.$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$hkl : l = 2n$
2	a $mmm.$	$0, 0, 0$	$0, 0, \frac{1}{2}$			$hkl : l = 2n$

Symmetry of special projections

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

Along $[100]$ $p2mm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, 0, 0$

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

(Continued on preceding page)