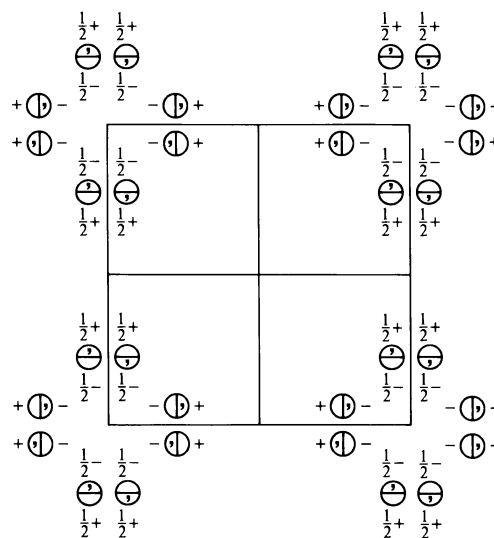
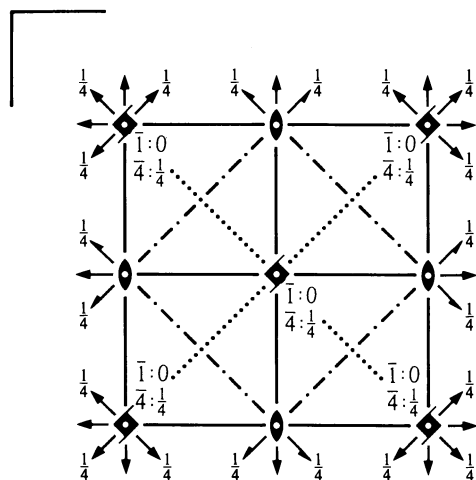


$P4_2/mmc$ 
 $D_{4h}^9$ 
 $4/mmm$ 

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**  $0 \leq x \leq \frac{1}{2}$ ;  $0 \leq y \leq \frac{1}{2}$ ;  $0 \leq z \leq \frac{1}{4}$ 
**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 $x,x,\frac{1}{4}$                      | (8) 2 $x,\bar{x},\frac{1}{4}$                |
| (9) $\bar{1}$ $0,0,0$ | (10) $m$ $x,y,0$ | (11) $\bar{4}^+$ $0,0,z$ ; $0,0,\frac{1}{4}$ | (12) $\bar{4}^-$ $0,0,z$ ; $0,0,\frac{1}{4}$ |
| (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**

- |          |                                 |                            |
|----------|---------------------------------|----------------------------|
| <b>I</b> | [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

- |            |  |
|------------|--|
| <b>IIb</b> | [2] $C4_2/emc$ ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_2/nm$ , 138); [2] $C4_2/mmd$ ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_2/mnm$ , 136); |
|            | [2] $C4_2/emd$ ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_2/nm$ , 134); [2] $C4_2/mmc$ ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_2/mcm$ , 132)  |

**Maximal isomorphic subgroups of lowest index**

- |            |   |
|------------|---|
| <b>IIc</b> | [3] $P4_2/mmc$ ( $\mathbf{c}' = 3\mathbf{c}$ ) (131); [9] $P4_2/mmc$ ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (131) |
|------------|---|

**Minimal non-isomorphic supergroups**

- |           |  |
|-----------|--|
| <b>I</b>  | [3] $Pm\bar{3}n$ (223)   |
| <b>II</b> | [2] $C4_2/mmc$ ( $P4_2/mcm$ , 132); [2] $I4/mmm$ (139); [2] $P4/mmm$ ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (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
16 <i>r</i> 1	(1) $x, y, z$ (2) $\bar{x}, \bar{y}, z$ (3) $\bar{y}, x, z + \frac{1}{2}$ (4) $y, \bar{x}, z + \frac{1}{2}$ (5) $\bar{x}, y, \bar{z}$ (6) $x, \bar{y}, \bar{z}$ (7) $y, x, \bar{z} + \frac{1}{2}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (10) $x, y, \bar{z}$ (11) $y, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y}, x, \bar{z} + \frac{1}{2}$ (13) $x, \bar{y}, z$ (14) $\bar{x}, y, z$ (15) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (16) $y, x, z + \frac{1}{2}$	General: $hhl : l = 2n$ $00l : l = 2n$  Special: as above, plus no extra conditions
8 <i>q</i> $m..$	$x, y, 0$ $\bar{x}, y, 0$ $\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	no extra conditions
8 <i>p</i> $.m.$	$\frac{1}{2}, y, z$ $\frac{1}{2}, y, \bar{z}$ $\bar{y}, \frac{1}{2}, z + \frac{1}{2}$ $y, \frac{1}{2}, \bar{z} + \frac{1}{2}$	no extra conditions
8 <i>o</i> $.m.$	$0, y, z$ $0, y, \bar{z}$ $\bar{y}, 0, z + \frac{1}{2}$ $y, 0, \bar{z} + \frac{1}{2}$	no extra conditions
8 <i>n</i> $..2$	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x}, \frac{3}{4}$ $\bar{x}, x, \frac{3}{4}$ $x, \bar{x}, \frac{1}{4}$	$hkl : l = 2n$
4 <i>m</i> $m2m.$	$x, \frac{1}{2}, 0$ $\bar{x}, \frac{1}{2}, 0$ $\frac{1}{2}, x, \frac{1}{2}$ $\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>l</i> $m2m.$	$x, 0, \frac{1}{2}$ $\bar{x}, 0, \frac{1}{2}$ $0, x, 0$ $0, \bar{x}, 0$	no extra conditions
4 <i>k</i> $m2m.$	$x, \frac{1}{2}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, x, 0$ $\frac{1}{2}, \bar{x}, 0$	no extra conditions
4 <i>j</i> $m2m.$	$x, 0, 0$ $\bar{x}, 0, 0$ $0, x, \frac{1}{2}$ $0, \bar{x}, \frac{1}{2}$	no extra conditions
4 <i>i</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 <i>h</i> $2mm.$	$\frac{1}{2}, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
4 <i>g</i> $2mm.$	$0, 0, z$ $0, 0, z + \frac{1}{2}$ $0, 0, \bar{z}$ $0, 0, \bar{z} + \frac{1}{2}$	$hkl : l = 2n$
2 <i>f</i> $\bar{4}m2$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, \frac{3}{4}$	$hkl : l = 2n$
2 <i>e</i> $\bar{4}m2$	$0, 0, \frac{1}{4}$ $0, 0, \frac{3}{4}$	$hkl : l = 2n$
2 <i>d</i> $mmm.$	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, 0$	$hkl : h + k + l = 2n$
2 <i>c</i> $mmm.$	$0, \frac{1}{2}, 0$ $\frac{1}{2}, 0, \frac{1}{2}$	$hkl : h + k + l = 2n$
2 <i>b</i> $mmm.$	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$hkl : l = 2n$
2 <i>a</i> $mmm.$	$0, 0, 0$ $0, 0, \frac{1}{2}$	$hkl : l = 2n$

**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)