

$I4_1md$

$C_{4v}^{11}$

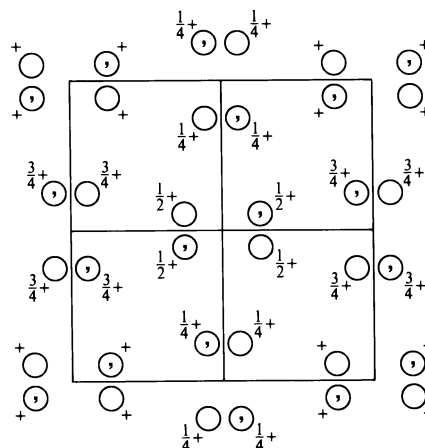
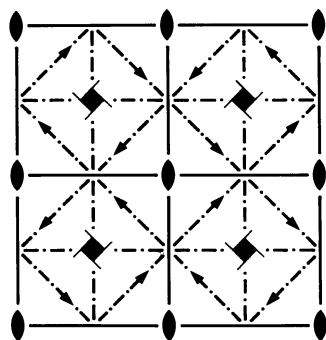
$4mm$

Tetragonal

No. 109

$I4_1md$

Patterson symmetry  $I4/mmm$



Origin on  $2mm$  on  $2m1$

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

For  $(0,0,0)+$  set

- |                 |  |   |  |
|-----------------|--|---|--|
| (1) 1           | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$                 | (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$          |
| (5) $m$ $x,0,z$ | (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ | (7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$ |

For  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$  set

- |  |                 |   |  |
|--|-----------------|---|--|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$         | (2) $2$ $0,0,z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$                  | (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$           |
| (5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ | (6) $m$ $0,y,z$ | (7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$ | (8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$ |

**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16 <i>c</i> 1	(1) $x,y,z$ (5) $x,\bar{y},z$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $y+\frac{1}{2},x,z+\frac{3}{4}$	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : 2h+l=4n$ $00l : l=4n$ $h00 : h=2n$ $h\bar{h}0 : h=2n$
8 <i>b</i> . <i>m</i> .	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$	Special: as above, plus no extra conditions
4 <i>a</i> 2 <i>m</i> <i>m</i> .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			$hkl : l=2n+1$ or $2h+l=4n$

**Symmetry of special projections**

Along [001]  $p4gm$

$$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$$

Origin at  $\frac{1}{4},\frac{1}{4},z$

Along [100]  $c1m1$

$$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}$$

Origin at  $x,0,0$

Along [110]  $c1m1$

$$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c}$$

Origin at  $x,x,0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I4_111$ ( $I4_1, 80$ )	(1; 2; 3; 4)+
	[2] $I2m1$ ( $Imm2, 44$ )	(1; 2; 5; 6)+
	[2] $I21d$ ( $Fdd2, 43$ )	(1; 2; 7; 8)+

**IIa** none

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3]  $I4_1md$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (109); [9]  $I4_1md$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (109)

**Minimal non-isomorphic supergroups**

**I** [2]  $I4_1/amd$  (141)

**II** [2]  $C4_2md$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P4_2nm, 102$ )