

$I4_122$

D_4^{10}

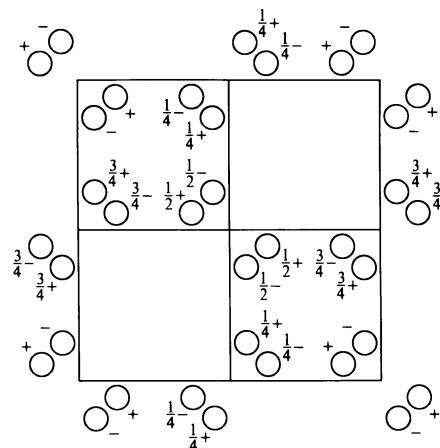
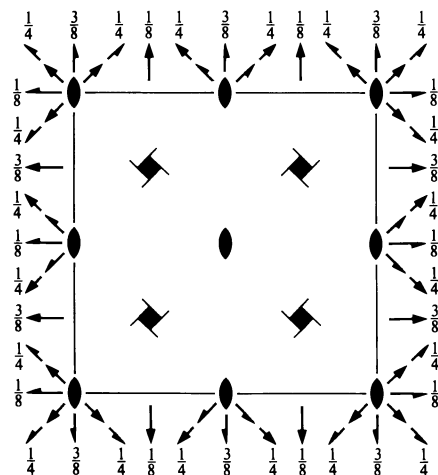
422

Tetragonal

No. 98

$I4_122$

Patterson symmetry $I4/mmm$



Origin at 222 at 212

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{8}$

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) $2 \frac{1}{4}, y, \frac{3}{8}$ | (6) $2 x, \frac{1}{4}, \frac{1}{8}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ | (8) $2 x, \bar{x}, 0$ |

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) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{8}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{3}{8}$ | (7) $2 x, x, 0$ | (8) $2 x, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |

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>g</i> 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$ (6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$ (7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) \bar{y},\bar{x},\bar{z}	$hkl : h+k+l=2n$ $hk0 : h+k=2n$ $0kl : k+l=2n$ $hhl : l=2n$ $00l : l=4n$ $h00 : h=2n$
8 <i>f</i> .2.	$x,\frac{1}{4},\frac{1}{8}$ $\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$ $\frac{3}{4},\bar{x},\frac{7}{8}$	$hhl : l=4n$
8 <i>e</i> ..2	$\bar{x},x,0$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},x,\frac{3}{4}$	$0kl : k=2n+1$ or $l=4n$
8 <i>d</i> ..2	$x,x,0$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x},x+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$	$0kl : k=2n+1$ or $l=4n$
8 <i>c</i> 2..	$0,0,z$ $0,\frac{1}{2},z+\frac{1}{4}$ $\frac{1}{2},0,\bar{z}+\frac{3}{4}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$hkl : l=2n+1$ or $2h+l=4n$
4 <i>b</i> 2.22	$0,0,\frac{1}{2}$ $0,\frac{1}{2},\frac{3}{4}$	$hkl : l=2n+1$ or $2h+l=4n$
4 <i>a</i> 2.22	$0,0,0$ $0,\frac{1}{2},\frac{1}{4}$	$hkl : l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$

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

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

Along [100] $c2mm$

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

Origin at $x,0,\frac{3}{8}$

Along [110] $p2mm$

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

Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2] $I4_1$ 11 ($I4_1$, 80)	(1; 2; 3; 4)+
	[2] $I2$ 21 ($I2$, 2_1 , 24)	(1; 2; 5; 6)+
	[2] $I2$ 12 ($F222$, 22)	(1; 2; 7; 8)+
IIa	[2] $P4_3$ 2,2 (96)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_3$ 22 (95)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_1$ 2,2 (92)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $P4_1$ 22 (91)	1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1$ 22 ($\mathbf{c}' = 3\mathbf{c}$) (98); [9] $I4_1$ 22 ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) (98)

Minimal non-isomorphic supergroups

I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $F4_1$ 32 (210); [3] $I4_1$ 32 (214)

II [2] $C4_2$ 22 ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P4_2$ 22, 93)