

$I4_122$

D_4^{10}

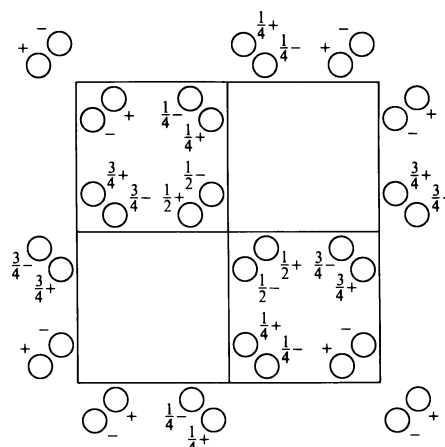
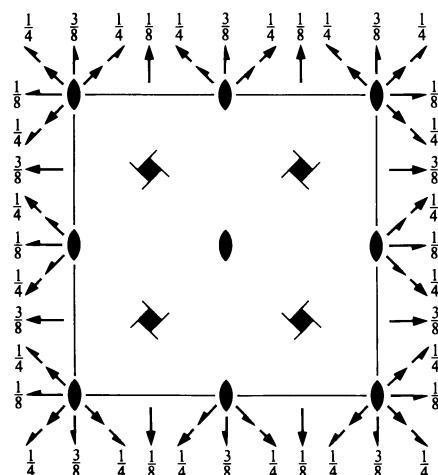
422

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

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

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

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
16	<i>g</i>	1	(0,0,0)+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + (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) $\bar{y}, \bar{x}, \bar{z}$	General: $hkl: h + k + l = 2n$ $hk0: h + k = 2n$ $0kl: k + l = 2n$ $hhl: l = 2n$ $00l: l = 4n$ $h00: h = 2n$
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] $p4mm$ $\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z$ $\frac{1}{4}, \frac{1}{4}, z$