

$P4_3 2_1 2$

D_4^8

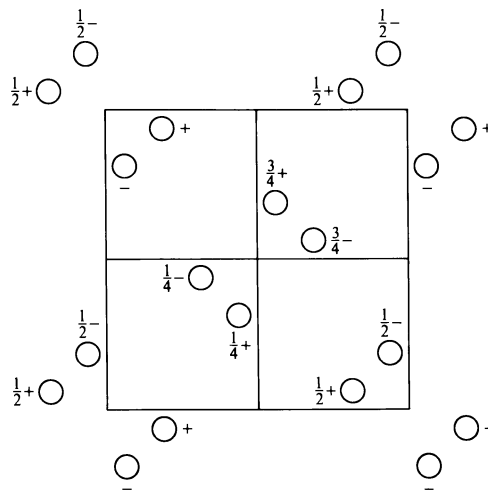
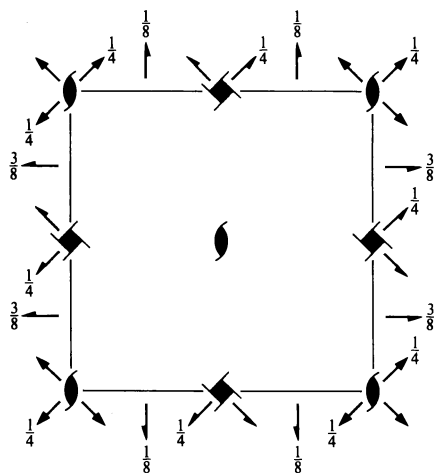
422

Tetragonal

No. 96

$P4_3 2_1 2$

Patterson symmetry $P4/mmm$



Origin on $2[110]$ at $2_1 1(1,2)$

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

Symmetry operations

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

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>b</i> 1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{3}{4}$	(4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{4}$	$00l : l = 4n$ $h00 : h = 2n$
	(5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(7) y, x, \bar{z}	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$	Special: as above, plus
4 <i>a</i> .. 2	$x, x, 0$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$	$0kl : l = 2n + 1$ or $2k + l = 4n$

Symmetry of special projections

Along [001] $p4gm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0, \frac{1}{2}, z$

Along [100] $p2gg$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, \frac{1}{4}, \frac{1}{8}$

Along [110] $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x, x, 0$

Maximal non-isomorphic subgroups

I [2] $P4_3 11 (P4_3, 78)$ 1; 2; 3; 4
 [2] $P2_1 12 (C222_1, 20)$ 1; 2; 7; 8
 [2] $P2_1 2_1 1 (P2_1 2_1 2_1, 19)$ 1; 2; 5; 6

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $P4_1 2_1 2 (\mathbf{c}' = 3\mathbf{c})$ (92); [5] $P4_3 2_1 2 (\mathbf{c}' = 5\mathbf{c})$ (96); [9] $P4_3 2_1 2 (\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})$ (96)

Minimal non-isomorphic supergroups

I [3] $P4_3 32$ (212)

II [2] $C4_3 22 (P4_3 22, 95)$; [2] $I4_1 22$ (98); [2] $P4_2 2_1 2 (\mathbf{c}' = \frac{1}{2}\mathbf{c})$ (94)