

$P4_322$

$D_4^7$

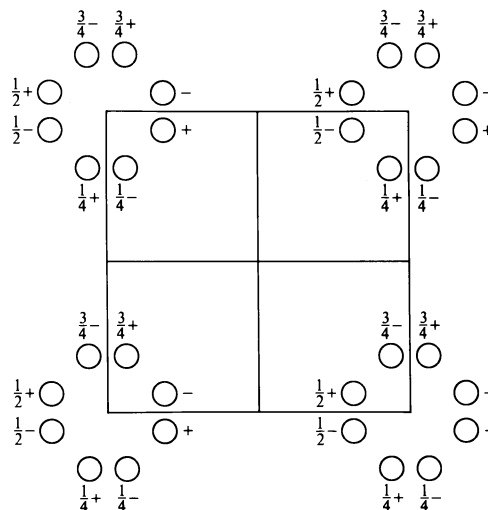
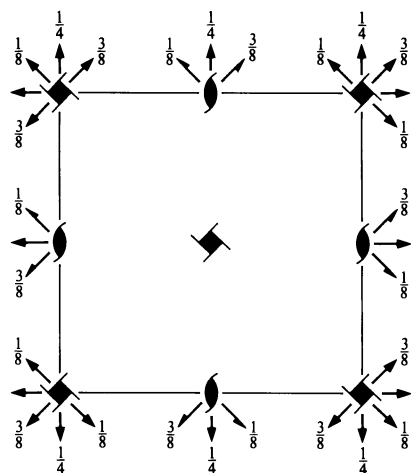
422

Tetragonal

No. 95

$P4_322$

Patterson symmetry  $P4/mmm$



Origin on  $2[010]$  at  $4_3(1,2)1$

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) $4^+(0,0,\frac{3}{4})$ $0,0,z$ | (4) $4^-(0,0,\frac{1}{4})$ $0,0,z$ |
| (5) $2_0,y,0$ | (6) $2_x,0,\frac{1}{4}$          | (7) $2_x,x,\frac{1}{8}$            | (8) $2_x,\bar{x},\frac{3}{8}$      |

**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
8 <i>d</i> 1	(1) $x, y, z$ (5) $\bar{x}, y, \bar{z}$	(2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{3}{4}$ (7) $y, x, \bar{z} + \frac{1}{4}$	(4) $y, \bar{x}, z + \frac{1}{4}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{3}{4}$	General: $00l : l = 4n$  Special: as above, plus
4 <i>c</i> . . 2	$x, x, \frac{5}{8}$	$\bar{x}, \bar{x}, \frac{1}{8}$	$\bar{x}, x, \frac{3}{8}$	$x, \bar{x}, \frac{7}{8}$	$0kl : l = 2n + 1$ or $l = 4n$
4 <i>b</i> . 2 .	$\frac{1}{2}, y, 0$	$\frac{1}{2}, \bar{y}, \frac{1}{2}$	$\bar{y}, \frac{1}{2}, \frac{3}{4}$	$y, \frac{1}{2}, \frac{1}{4}$	$hhl : l = 2n + 1$ or $l = 4n$
4 <i>a</i> . 2 .	$0, y, 0$	$0, \bar{y}, \frac{1}{2}$	$\bar{y}, 0, \frac{3}{4}$	$y, 0, \frac{1}{4}$	$hhl : l = 2n + 1$ or $l = 4n$

**Symmetry of special projections**

Along [001]  $p4mm$   
 $\mathbf{a}' = \mathbf{a}$     $\mathbf{b}' = \mathbf{b}$   
Origin at  $0, 0, z$

Along [100]  $p2gm$   
 $\mathbf{a}' = \mathbf{b}$     $\mathbf{b}' = \mathbf{c}$   
Origin at  $x, 0, \frac{1}{4}$

Along [110]  $p2gm$   
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$     $\mathbf{b}' = \mathbf{c}$   
Origin at  $x, x, \frac{1}{8}$

**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]  $P2_1 21$  ( $P222_1, 17$ )   1; 2; 5; 6

**IIa** none

**IIb** [2]  $C4_3 22_1$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_3 2_1 2, 96$ )

**Maximal isomorphic subgroups of lowest index**

**IIc** [2]  $C4_3 22$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) ( $P4_3 22, 95$ ); [3]  $P4_1 22$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (91); [5]  $P4_3 22$  ( $\mathbf{c}' = 5\mathbf{c}$ ) (95)

**Minimal non-isomorphic supergroups**

**I** none

**II** [2]  $I4_1 22$  (98); [2]  $P4_3 22$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) (93)