

$P4_122$

D_4^3

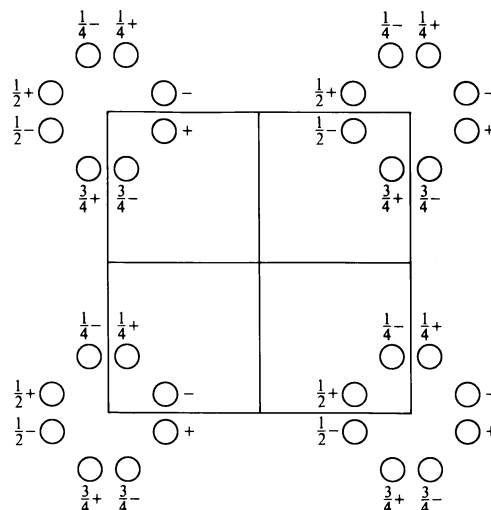
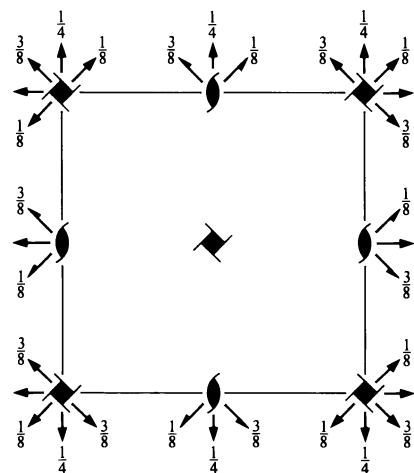
422

Tetragonal

No. 91

$P4_122$

Patterson symmetry $P4/mmm$



Origin on $2[010]$ at $4_1(1,2)1$

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

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

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 $x, x, \frac{3}{8}$

Maximal non-isomorphic subgroups

I [2] $P4_111$ ($P4_1$, 76) 1; 2; 3; 4
[2] $P2_121$ ($P222_1$, 17) 1; 2; 5; 6
[2] $P2_112$ ($C222_1$, 20) 1; 2; 7; 8

IIa none

IIb [2] $C4_122_1$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_12_12$, 92)

Maximal isomorphic subgroups of lowest index

IIc [2] $C4_122$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4_122$, 91); [3] $P4_322$ ($\mathbf{c}' = 3\mathbf{c}$) (95); [5] $P4_122$ ($\mathbf{c}' = 5\mathbf{c}$) (91)

Minimal non-isomorphic supergroups

I none

II [2] $I4_122$ (98); [2] $P4_122$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (93)